AR201-13323B

I U C L I D

D a t a S e t

Existing Chemical	ID: 13752-51-7
CAS No.	13752-51-7
CAS Name	N-oxydiethylenethiocarbamyl-N-oxydiethylenesulfenamide
EINECS No.	237-335-9
Producer Related Part	
Company:	
Creation date:	09-NOV-2000
Substance Related Part	
Company:	
Creation date:	09-NOV-2000
Memo:	Rubber and Plastic Additives (RAPA) HPV Panel
Printing date:	12-OCT-2001
Revision date:	
Date of last Update:	12-OCT-2001
Number of Pages:	28
Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: American Chemistry Council (formerly Chemical Manufacturers Association) Rubber and Plastic Additives (RAPA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States
Phone: 703-741-5600
Telefax: 703-741-6091

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Type: cooperating company
Name: Bayer Corporation
Country: United States

11-OCT-2001

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Country: United States

11-OCT-2001

Type: cooperating company
Name: Crompton Corporation
Country: United States

11-OCT-2001

Type: cooperating company
Name: Flexsys America L.P.
Country: United States

11-OCT-2001

Type: cooperating company
Name: Noveon, Inc (formerly BF Goodrich)
Country: United States

11-OCT-2001

Type: cooperating company
Name: R.T. Vanderbilt Company, Inc.
Country: United States

11-OCT-2001

Type: cooperating company
Name: The Goodyear Tire & Rubber Company
Country: United States

11-OCT-2001

Type: cooperating company
Name: The Lubrizol Corporation
Country: United States

11-OCT-2001

Type: cooperating company
Name: UOP, LLC.
Country: United States

11-OCT-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: solid
Purity: 95 - 99 % w/w
25-APR-2001

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

Morpholine, 4-[(morpholinothiocarbonyl)thio]-
25-APR-2001

Cure-Rite® 18
25-APR-2001

Good-Rite® 3030x18
25-APR-2001

1.3 Impurities

CAS-No: 729-46-4
EINECS-No:
EINECS-Name: Dimorpholine Thiuram Disulfide
Contents: < 5 % w/w
25-APR-2001

CAS-No: 34986-62-4
EINECS-No:
EINECS-Name: [4-(4'-morpholinodithion) thioxomethyl-morpholine]
Contents: < .5 % w/w
25-APR-2001

CAS-No: 110-91-8
EINECS-No: 203-815-1
EINECS-Name: morpholine
Contents: < .02 % w/w
25-APR-2001

CAS-No: 59-89-2
EINECS-No:
EINECS-Name: N-nitrosomorpholine
Contents: < .005 % w/w
25-APR-2001

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern
-

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value:	124.3 degree C
Method:	other: (calculated) MPBPWIN (v1.31)
Year:	1999
GLP:	no
Testsubstance:	other TS: molecular structure
Remark:	Comparable to BFG MSDS data of >/= 132 °C
Result:	Melting Point: 251.84 deg C (Adapted Joback Method) Melting Point: 92.44 deg C (Gold and Ogle Method) Mean Melt Pt : 172.14 deg C (Joback; Gold,Ogle Methods) Selected MP: 124.32 deg C (Weighted Value)
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint

11-OCT-2001 (1)

2.2 Boiling Point

Value:	353 degree C
Method:	other: (calculated) MPBPWIN (v1.31) - Adapted Stein and Brown Method
Year:	1999
GLP:	no
Testsubstance:	other TS: molecular structure
Remark:	BFGoodrich MSDS indicates Not Applicable
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint

11-OCT-2001 (1)

2.3 Density

Type:	density
Value:	.6 g/cm3
Method:	other: historical data
Testsubstance:	as prescribed by 1.1 - 1.4

25-APR-2001 (2)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: .0000153 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 352.97 deg C (estimated))
(Using MP: 124.32 deg C (estimated))
VP: 5.17E-006 mm Hg (Antoine Method)
VP: 1.15E-005 mm Hg (Modified Grain Method)
VP: 2.32E-005 mm Hg (Mackay Method)
Selected VP: 1.15E-005 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
11-OCT-2001 (1)

2.5 Partition Coefficient

log Pow: -.84
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
11-OCT-2001 (1)

2.6.1 Water Solubility

Value: 62.85 g/l at 25 degree C
Method: other: (calculated) WSKOW (v1.36)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Log Kow (estimated) : -0.84
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.84

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW +
Correction (used when Melting Point NOT available)

Correction(s):	Value
Amine, aliphatic	1.008
Multi-Nitrogen Type	-1.310

Log Water Solubility (in moles/L) : -0.597
Water Solubility at 25 deg C (mg/L): 6.285e+004

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
11-OCT-2001 (1)

2.6.2 Surface Tension
-

2.7 Flash Point
-

2.8 Auto Flammability

Value: 275 degree C
Remark: Self-Ignition Temperature
25-APR-2001 (2)

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .000000000002156 cm3/(molecule * sec)
Degradation: 50 % after .6 hour(s)
Method: other (calculated): AOP (v1.89):
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
11-OCT-2001 (1)

3.1.2 Stability in Water

See IUCLID data sets on CAS# 95-31-8; 102-77-2; 95-33-0; 4979-32-2

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air, water, soil, sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.00657	1.19	1000	1.47e-013
Water	50.2	900	1000	9.26e-015
Soil	49.7	900	1000	3.38e-013
Sediment	0.0927	3.6e+003	0	8.53e-015

Persistence Time: 763 hr
Reaction Time: 1.24e+003 hr
Advection Time: 1.99e+003 hr
Percent Reacted: 61.6
Percent Advected: 38.4
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint

11-OCT-2001 (1)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

See IUCLID data sets on CAS# 95-31-8; 102-77-2; 95-33-0; 4979-32-2

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation

Species: other: calculation
Exposure period:
Concentration:
BCF: 3.16
Elimination:
Method: other: BCF Program (v2.13)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Result: Log Kow (estimated) : -0.84
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: -0.84

Equation Used to Make BCF estimate:
Log BCF = 0.50
Correction(s): Correction Factors Not Used for Log Kow < 1

Estimated Log BCF = 0.500 (BCF = 3.162)
Accepted calculation method

11-OCT-2001 (1)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

See also IUCLID data sets on CAS# 95-31-8; 102-77-2; 95-33-0; 4979-32-2

Type:	other: calculation		
Species:	other: Fish		
Exposure period:	96 hour(s)		
Unit:	g/l	Analytical monitoring:	no
LC50:	86.036		
Method:	other: ECOSAR v0.99e		
Year:	1999	GLP:	no
Test substance:	other TS: molecular structure		
Remark:	Chemical may not be soluble enough to measure this predicted effect.		
Reliability:	(2) valid with restrictions Accepted calculation method		
Flag:	Critical study for SIDS endpoint		
11-OCT-2001			(1)

Type:	other: calculation		
Species:	other: Saltwater Fish		
Exposure period:	96 hour(s)		
Unit:	g/l	Analytical monitoring:	no
LC50:	4.992		
Method:	other: ECOSAR v0.99e		
Year:	1999	GLP:	no
Test substance:	other TS: molecular structure		
Remark:	Chemical may not be soluble enough to measure this predicted effect.		
Reliability:	(2) valid with restrictions Accepted calculation method		
Flag:	Critical study for SIDS endpoint		
11-OCT-2001			(1)

Type:	other: calculation		
Species:	other: Fish		
Exposure period:	14 day		
Unit:	g/l	Analytical monitoring:	no
LC50:	99.248		
Method:	other: ECOSAR v0.99e		
Year:	1999	GLP:	no
Test substance:	other TS: molecular structure		
Remark:	Chemical may not be soluble enough to measure this predicted effect.		
Reliability:	(2) valid with restrictions Accepted calculation method		
11-OCT-2001			(1)

4.2 Acute Toxicity to Aquatic Invertebrates

See also IUCLID data sets on CAS# 95-31-8; 102-77-2; 95-33-0; 4979-32-2

Type:	other: calculation
Species:	Daphnia sp. (Crustacea)
Exposure period:	48 hour(s)
Unit:	g/l Analytical monitoring: no
LC50 :	75.767
Method:	other: ECOSAR v0.99e
Year:	1999 GLP: no
Test substance:	other TS: molecular structure
Remark:	Chemical may not be soluble enough to measure this predicted effect.
Reliability:	(2) valid with restrictions
Flag:	Critical study for SIDS endpoint
11-OCT-2001	(1)

Type:	other: calculation
Species:	Mysidopsis bahia (Crustacea)
Exposure period:	96 hour(s)
Unit:	g/l Analytical monitoring: no
LC50 :	188
Method:	other: ECOSAR v0.99e
Year:	1999 GLP: no
Test substance:	other TS: molecular structure
Remark:	Chemical may not be soluble enough to measure this predicted effect.
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint
11-OCT-2001	(1)

Type:	other: calculation
Species:	Daphnia sp. (Crustacea)
Exposure period:	16 day
Unit:	mg/l Analytical monitoring: no
EC50:	1121
Method:	other: ECOSAR v0.99e
Year:	1999 GLP: no
Test substance:	other TS: molecular structure
Remark:	Chemical may not be soluble enough to measure this predicted effect.
Reliability:	(2) valid with restrictions Accepted calculation method
11-OCT-2001	(1)

4.3 Toxicity to Aquatic Plants e.g. Algae

See also IUCLID data sets on CAS# 95-31-8; 102-77-2; 95-33-0; 4979-32-2

Species:	other algae: green algae
Endpoint:	growth rate
Exposure period:	96 hour(s)
Unit:	g/l Analytical monitoring: no
EC50:	40.223
ChV :	0.779
Method:	other: ECOSAR v0.99e
Year:	GLP: no
Test substance:	other TS: molecular structure
Remark:	Chemical may not be soluble enough to measure this predicted effect.
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint

11-OCT-2001 (1)

4.4 Toxicity to Microorganisms e.g. Bacteria
-

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species:	other: fish
Endpoint:	other
Exposure period:	30 day
Unit:	mg/l Analytical monitoring: no
ChV :	7012
Method:	other: ECOSAR v0.99e
Year:	1999 GLP: no
Test substance:	other TS: molecular structure
Remark:	Chemical may not be soluble enough to measure this predicted effect.
Reliability:	(2) valid with restrictions Accepted calculation method

11-OCT-2001 (1)

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:	other: calculation
Species:	Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint:	mortality
Exposure period:	14 day
Unit:	other: ppm
LC50:	11449
Method:	other: ECOSAR v0.99e
Year:	1999 GLP: no
Test substance:	other TS: molecular structure
Remark:	Chemical may not be soluble enough to measure this predicted effect.
Reliability:	(2) valid with restrictions Accepted calculation method

11-OCT-2001 (1)

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type:	LD50
Species:	rat
Strain:	Sprague-Dawley
Sex:	
Number of Animals:	
Vehicle:	
Value:	5200 mg/kg bw
Method:	other: 40CFR Part 163.81-1
Year:	GLP: yes
Test substance:	other TS: Cure-Rite® 18, purity: not noted
Remark:	Rat/CD® Sprague-Dawley (Charles River) Discriminating dose: LD0 = 2,700 mg/kg
Reliability:	(1) valid without restriction GLP study, Meets National standards method
Flag:	Critical study for SIDS endpoint

11-OCT-2001 (3)

Type:	LD50
Species:	mouse
Strain:	CD-1
Sex:	male/female
Number of Animals:	
Vehicle:	
Value:	9000 mg/kg bw
Method:	other: 40CFR Part 163.81-1
Year:	GLP: yes
Test substance:	other TS: Cure-Rite® 18; purity: not noted
Remark:	Discriminating dose: LD0 = 4,050 mg/kg LD50 (95% conf. Limits) = 11,000 mg/kg (5,100-16,900 mg/kg) for males and 7,000 mg/kg (4,900-9,100 mg/kg) for females
Reliability:	(1) valid without restriction GLP study, Meets National standards method
Flag:	Critical study for SIDS endpoint

11-OCT-2001 (4)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	5110 mg/kg bw
Method:	other: Federal Hazardous Substances Act (Revised, Fed. Reg., September 17, 1964
Year:	1964 GLP: no
Test substance:	other TS: Good-Rite® 3030x18 (Cure-Rite® 18) ; purity: not noted
Remark:	Discriminating dose: LD0 = 1,000 mg/kg

Reliability: (2) valid with restrictions
25-APR-2001 (5)

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex:
Number of Animals:
Vehicle:
Value: 5000 mg/kg bw
Method: other: 40CFR Part 163.81-1
Year: GLP: yes
Test substance: other TS: Cure-Rite® 18; purity: not noted
Remark: Rat/CD® Sprague-Dawley (Taconic Farms)
Discriminating dose: LD0 = 2,700 mg/kg
Reliability: (1) valid without restriction
GLP study, Meets National standards method
11-OCT-2001 (3)

5.1.2 Acute Inhalation Toxicity

Type: LC0
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time: 1 hour(s)
Value: 164.4 mg/l
Method: other: Federal Hazardous Substances Act (Revised, Fed. Reg., September 17, 1964)
Year: 1964 GLP: no
Test substance: other TS: Good-Rite® 3030x18 (Cure-Rite® 18); purity: not noted
Remark: Test substances measured not analysed.
Reliability: (1) valid without restriction
Meets National standards method
Flag: Critical study for SIDS endpoint
11-OCT-2001 (5)

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rabbit
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	> 10000 mg/kg bw
Method:	other:) Federal Hazardous Substances Act (Revised, Fed. Reg., September 17, 1964)
Year:	1964 GLP: no
Test substance:	other TS: Good-Rite® 3030x18 (Cure-Rite® 18); purity: not noted
Reliability:	(1) valid without restriction Meets National standards method
Flag:	Critical study for SIDS endpoint

11-OCT-2001 (5)

5.1.4 Acute Toxicity, other Routes

-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

-

5.2.2 Eye Irritation

Species:	rabbit
Concentration:	
Dose:	
Exposure Time:	
Comment:	
Number of Animals:	
Result:	not irritating
EC classificat.:	
Method:	other: Section 1500.42, Federal Hazardous Substances Act Regulations, CFR 16, p. 125
Year:	GLP: yes
Test substance:	other TS: Cure-Rite® 18; purity: not noted
Result:	No positive scores; one animal had scores of "1" for redness and chemosis at day one.
Reliability:	(1) valid without restriction GLP study, Meets National standards method

11-OCT-2001 (6)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: other: Federal Hazardous Substances Act (Revised, Fed. Reg., September 17, 1964)
Year: 1964 GLP: no
Test substance: other TS: Good-Rite® 3030x18 (Cure-Rite® 18); purity: not noted
Reliability: (1) valid without restriction
Meets National standards method
11-OCT-2001 (5)

5.3 Sensitization
-

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 2 years
Frequency of treatment: continuous daily
Post. obs. period: none
Doses: 0, 20, 60, 200, or 600 ppm
Control Group: yes, concurrent no treatment
NOAEL: 200 ppm
LOAEL: 600 ppm
Method: EPA OPP 82-5
Year: GLP: yes
Test substance: other TS: Commercial Cure-Rite® 18; purity: 96.8%
Result: A compound related increase in urothelial tumors, kidney weights, non-neoplastic urinary tract abnormalities, and rales was observed in the high dose (600 ppm) males and females. Body weights also were significantly lower in the high dose in the high dose males and females. No compound-related effects on hematology, clinical chemistry, or urinalysis were noted.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
11-OCT-2001 (7)

5.5 Genetic Toxicity 'in Vitro'

Type:	Bacterial reverse mutation assay
System of testing:	Salmonella typhimurium strains TA-1535, TA-1537, TA-1538, TA-98, TA-100
Concentration:	0.5 to 1,000 ug/plate
Cytotoxic Conc.:	With metabolic activation: 0.5 to 100 ug/plate (little to no toxicity) Without metabolic activation: 0.5 to 100 ug/plate (little to no toxicity)
Metabolic activation:	with and without
Result:	negative
Method:	other: according to other: according to Ames et al (1975) Mutation Res. 31:347-364; McCann et al. (1975) Proc. Nat. Acad. Sci. 72:5135-5139
Year:	1975 GLP: no data
Test substance:	other TS: Commercial Cure-Rite® 18 (Purified); purity: 97.5%
Remark:	Signed QA assurance statement provided
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag:	Critical study for SIDS endpoint

12-OCT-2001 (8) (9)

Type:	Bacterial reverse mutation assay
System of testing:	Escherichia coli strain WP2urvA-
Concentration:	0.5 to 1,000 ug/plate
Cytotoxic Conc.:	With metabolic activation: 0.5 to 100 ug/plate (little to no toxicity) Without metabolic activation: 0.5 to 100 ug/plate (little to no toxicity)
Metabolic activation:	with and without
Result:	negative
Method:	other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year:	1983 GLP: no data
Test substance:	other TS: Cure-Rite® 18 (purified), purity: 97.5%
Remark:	Signed QA assurance statement provided
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag:	Critical study for SIDS endpoint

12-OCT-2001 (8) (9)

Type: Cytogenetic assay
System of testing: Chinese Hamster Ovary (CHO) Cells
Concentration: 2.500 to 20.000 ug/ml
Cytotoxic Conc.: concentration used based on mouse lymphoma L5178Y cells
Metabolic activation: with and without
Result: positive
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Cure-Rite® 18 (purified); purity = 97.5%.
Remark: Signed QA assurance statement provided
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
12-OCT-2001 (8) (10)

Type: DNA damage and repair assay
System of testing: Escherichia coli strains W3110 (pol A+) and W3078 (pol A-)
Concentration: 100 to 5,000 ug/plate
Cytotoxic Conc.: With metabolic activation: 0.5 to 100 ug/plate (little or no toxicity) Without metabolic activation: 0.5 to 100 ug/plate (little or no toxicity)
Metabolic activation: with and without
Result: positive
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Cure-Rite® 18.(purified); purity: 97.5%
Remark: Signed QA assurance statement provided
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
12-OCT-2001 (8) (9)

Type: Mammalian cell gene mutation assay
System of testing: BALB 3T3 Mouse Cells
Concentration: 0.01000 to 0.20000 ug/ml
Cytotoxic Conc.: 0.488 ug/ml
Metabolic activation: without
Result: positive
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Cure-Rite® 18 (purified); purity = 97.5%.

Remark: Precipitation conc: >250 ug/ml
Signed QA assurance statement provided.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
12-OCT-2001 (8) (11)

Type: Mouse lymphoma assay
System of testing: Mouse Lymphoma cell line L5178Y TK+/-
Concentration: 1.250 to 25.0 ug/ml
Cytotoxic Conc.: With metabolic activation: Percent relative growth was 64.9% at 1.560 ug/ml and 5.2% at 25.0 ug/ml
Without metabolic activation: Percent relative growth was 29.7% at 1.250 ug/ml and 7.7-11.2% at 5.0-20.0 ug/ml
Metabolic activation: with and without
Result: positive
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Cure-Rite® 18 (purified); purity = 97.5%.
Remark: Precipitation conc: >250 ug/ml
Signed QA assurance statement provided.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
12-OCT-2001 (8) (9)

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium strains TA-1535, TA-1537, TA-1538, TA-98, TA-100
Concentration: 0.5 to 5,000 ug/plate
Cytotoxic Conc.: With metabolic activation: 0.5 to 100 ug/plate (little to no toxicity)
Without metabolic activation: 0.5 to 100 ug/plate (little to no toxicity)
Metabolic activation: with and without
Result: negative
Method: other: according to Ames et al (1975) Mutation Res. 31:347-364; McCann et al. (1975) Proc. Nat. Acad. Sci. 72:5135-5139
Year: 1975 GLP:
Test substance: other TS: Commercial Cure-Rite® 18, purity: 95.6%
Remark: Signed QA assurance statement provided
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (9)

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium strains TA-1535, TA-1537, TA-1538, TA-98, TA-100 and Saccharomyces strain D4
Concentration: 0.5 to 1,000 ug/plate
Cytotoxic Conc.: With metabolic activation: 1000 ug/plate (TA-98); 1000 ug/plate, 500 ug/plate, and 100 ug/plate (D4)
Without metabolic activation: 1000 ug/plate (TA-98); 1000 ug/plate, 500 ug/plate, and 100 ug/plate (D4)
Metabolic activation: with and without
Result: negative
Method: other: according to Ames et al (1975) Mutation Res. 31:347-364; McCann et al. (1975) Proc. Nat. Acad. Sci. 72:5135-5139
Year: 1975 GLP:
Test substance: other TS: Commercial Cure-Rite® 18; purity: not noted
Remark: QA assurance statement provided.
Saccharomyces strain D4 not reported in referenced publication.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (9)

Type: Bacterial reverse mutation assay
System of testing: Escherichia coli strain WP2urvA
Concentration: 0.5 to 1,000 ug/plate
Cytotoxic Conc.: With metabolic activation: 0.5 to 100 ug/plate (little or no toxicity) Without metabolic activation: 0.5 to 100 ug/plate (little or no toxicity)
Metabolic activation: with and without
Result: negative
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Commercial Cure-Rite® 18, purity: 95.6%
Remark: Signed QA assurance statement provided
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (9)

Type: Cytogenetic assay
System of testing: Chinese Hamster Ovary (CHO) Cells
Concentration: 0.313 to 5.000 ug/ml
Cytotoxic Conc.: concentration used based on mouse lymphoma L5178Y cells
Metabolic activation: with and without
Result:
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Commercial Cure-Rite® 18; purity = 95.6%.
Remark: Signed QA assurance statement provided
Result: Genotoxic effects:With metabolic activation: negative Without metabolic activation: positive
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (10)

Type: DNA damage and repair assay
System of testing: Escherichia coli strains W3110 (pol A+) and W3078 (pol A-)
Concentration: 100 to 5,000 ug/plate
Cytotoxic Conc.: With metabolic activation: 0.5 to 100 ug/plate (little or no toxicity) Without metabolic activation: 0.5 to 100 ug/plate (little or no toxicity)
Metabolic activation: with and without
Result: positive
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Commercial Cure-Rite® 18, purity: 95.6%
Remark: Signed QA assurance statement provided
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (9)

Type: Mammalian cell gene mutation assay
System of testing: BALB 3T3 Mouse Cells
Concentration: 0.05000 to 0.10000 ug/ml
Cytotoxic Conc.: 0.488 ug/ml
Metabolic activation: without
Result: negative
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Commercial Cure-Rite® 18; purity = 95.6%.

Remark: Signed QA assurance statement provided
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (11)

Type: Mammalian cell gene mutation assay
System of testing: BALB 3T3 Mouse Cells
Concentration: 0.00625 to 0.10000 ug/ml
Cytotoxic Conc.: 0.244 ug/ml
Metabolic activation: without
Result: positive
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Commercial Cure-Rite® 18, purity: Not noted
Remark: Weakly active.
Signed QA assurance statement provided.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (11)

Type: Mouse lymphoma assay
System of testing: Mouse Lymphoma cell line L5178Y TK+/-
Concentration: 0.313 to 35.0 ug/ml
Cytotoxic Conc.: With metabolic activation: Percent relative growth was 78.1% at 20.0 ug/ml and 5.7% at 35.0 ug/ml
Without metabolic activation:Percent relative growth was 25.6% at 0.313 ug/ml and 3.8% at 1.880 ug/ml
Metabolic activation: with and without
Result: positive
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Commercial Cure-Rite® 18; purity = 95.6%.
Remark: Weakly active.
Signed QA assurance statement provided.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (9)

Type: Mouse lymphoma assay
System of testing: Mouse Lymphoma cell line L5178Y TK+/-
Concentration: 0.313 to 50.0 ug/ml
Cytotoxic Conc.: With metabolic activation: Percent relative growth was 43.2% at 12.50 ug/ml and 4.2% at 50.0 ug/ml
Without metabolic activation: Percent relative growth was 80.9% at 0.313 ug/ml and 7.9% at 1.880 ug/ml
Metabolic activation: with and without
Result:
Method: other: according to Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215
Year: 1983 GLP:
Test substance: other TS: Commercial Cure-Rite® 18; purity: Not noted
Remark: Precipitation conc: 1250 ug/ml
Signed QA assurance statement provided.
Result: With metabolic activation: weakly active
Without metabolic activation: negative
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
12-OCT-2001 (8) (9)

5.6 Genetic Toxicity 'in Vivo'

Type: Dominant lethal assay
Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 56 consecutive days to males
Doses: 0, 6.25, 12.5, or 25 mg/kg. (0.25 mg/kg triethylenemelamine positive control)
Result: negative
Method: other: according to Hinderer, R.K., M. Knickerbocker, and F.J. Koschier (1982) Toxicol. Appl. Pharmacol. 62:335-341.
Year: 1982 GLP: yes
Test substance: other TS: Commercial Cure-Rite® 18; Purity = 95.6%
Result: A significant depression in body weight gain was observed in the males administered the highest dose. Similar pregnancy rates were observed in all test groups compared with the controls. No evidence of dominant lethal mutations were observed in the test groups. In the TEM positive controls, the number of implantation sites and preimplantation loses were significantly decreased, and the number of early fetal deaths per pregnant female were significantly elevated.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
12-OCT-2001 (12)

5.7 Carcinogenicity

Species:	rat		Sex: male/female
Strain:	Sprague-Dawley		
Route of admin.:	oral feed		
Exposure period:	2 years		
Frequency of treatment:	continuous daily		
Post. obs. period:	none		
Doses:	0, 20, 60, 200, or 600 ppm		
Result:			
Control Group:	yes, concurrent no treatment		
Method:	other: according to Hinderer, R.K., G.R. Lankas, A.L. Knezevich, and C.S. Auletta (1986). Toxicol. Appl. Pharmacol. 82:521-531		
Year:	1986	GLP:	
Test substance:	other TS: Commercial Cure-Rite® 18; purity = 96.8%		
Result:	A compound related increase in urothelial tumors, kidney weights, non-neoplastic urinary tract abnormalities, and rales was observed in the high dose males and females. Body weights also were significantly lower in the high dose males and females. No compound-related effects on hematology, clinical chemistry, or urinalysis were noted.		
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment		
Flag:	Critical study for SIDS endpoint		

12-OCT-2001 (7)

5.8 Toxicity to Reproduction

Type:	Fertility		
Species:	rat		Sex: male/female
Strain:	Sprague-Dawley		
Route of admin.:	oral feed		
Exposure Period:	12 weeks		
Frequency of treatment:	daily		
Premating Exposure Period			
male:	Males were sacrificed over a 6-7 day period following the 21-day mating period.		
Duration of test:	12 weeks		
Doses:	0, 60, 200, or 600 ppm.		
Control Group:	yes, concurrent no treatment		
NOAEL Parental:	200 ppm		
NOAEL F1 Offspr.:	600 ppm		
Method:	other: according to Hinderer, R.K., B.Y. Cockrell, S.M. Debanne, and P.T. Goad. (1987). Fund. Appl. Toxicol. 9:763-772.		
Year:	1987	GLP: yes	
Test substance:	other TS: Commercial Cure-Rite® 18; purity = 98.0%.		
Result:	NOEL Parental: 200 ppm based on a slight, but generally not statistically significant body weight reduction at 600 ppm		

No evidence of a compound-related effect on mating, fertility, gestation length, number of implants or live births, pup growth, or survival was observed.
No morphological changes in the testes from the high dose males was observed by either light or electron microscopy.

General parental toxicity: A slight but generally nonstatistically significant decrease in body weights in the test males.

Toxicity to offspring: None

Reliability: (1) valid without restriction
GLP study, Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag: Critical study for SIDS endpoint

12-OCT-2001 (13)

5.9 Developmental Toxicity/Teratogenicity

See IUCLID data sets on CAS# 95-31-8; 102-77-2; 95-33-0; 4979-32-2

5.10 Other Relevant Information

-

5.11 Experience with Human Exposure

-

(1) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

(2) BFGoodrich MSDS

(3) Bio/dynamics Inc., East Millstone, NJ (1980) Project #6216-80

(4) Bio/dynamics Inc., East Millstone, NJ (1980)

(5) Hill Top Research, Inc., Miamiville, Ohio (1971)

(6) Biosearch Inc, Philadelphia, PA(1981)

(7) Hinderer, R.K., G.R. Lankas, A.L. Knezevich, and C.S. Auletta (1986). Toxicol. Appl. Pharmacol. 82:521-531

(8) Hinderer, R.K., B. Myhr, D.R. Jagannath, S.M. Galloway, S.W. Mann, J.C.Riddle, and D.J. Brusick (1983) Environ. Mutagen. 5:193-215

(9) Litton Bionetics, Inc Report Project Number 20988 (1979)

(10) Litton Bionetics, Inc Report Project Number 20990 (1979)

(11) Litton Bionetics, Inc Report Project Number 20992 (1980)

(12) Hinderer, R.K., M. Knickerbocker, and F.J. Koschier (1982). Toxicol. Appl. Pharmacol. 62:335-341.

(13) Hinderer, R.K., B.Y. Cockrell, S.M. Debanne, and P.T. Goad. (1987). Fund. Appl. Toxicol. 9:763-772.

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 4979-32-2
CAS No.	4979-32-2
EINECS Name	N,N-dicyclohexylbenzothiazole-2-sulphenamide
EINECS No.	225-625-8
TSCA Name	2-Benzothiazolesulfenamide, N,N-dicyclohexyl-
Molecular Formula	C19H26N2S2

Producer Related Part	
Company:	
Creation date:	26-APR-2001

Substance Related Part	
Company:	
Creation date:	26-APR-2001

Memo:	Data for RAPA Sulfenamide Accelerators category

Printing date:	18-OCT-2001
Revision date:	
Date of last Update:	18-OCT-2001

Number of Pages:	28

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information
-

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: solid
Purity: >= 95 % w/w
Remark: cooperating companies:
Bayer Antwerpen N.V., Belgium
AKZO Chemicals, Netherlands
Monsanto Europe N.V., Belgium
26-APR-2001

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

N,N-dicyclohexyl-2-benzothiazolesulfenamide
26-APR-2001

Sanotcure DCBS
Source: Bayer AG Leverkusen
07-JUN-1994

Vulkacit DZ
Source: Bayer AG Leverkusen
07-JUN-1994

1.3 Impurities
-

1.4 Additives

CAS-No:
EINECS-No:
EINECS-Name:
Remark: Additives may be contained in the substance as marketed in order to reduce dust formation during use.
26-APR-2001

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern

Type: type
Category: Use resulting in inclusion into or onto matrix
26-APR-2001

Type: industrial
Category: Polymers industry
Source: Bayer AG Leverkusen
26-MAY-1994

Type: use
Category: Vulcanizing agents
Source: Bayer AG Leverkusen
26-MAY-1994

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value: >= 96 degree C
Decomposition: no
Sublimation: no
Method: other
Year: 1982
GLP: no
Remark: sample of technical purity
Source: Bayer AG Leverkusen
30-APR-1992 (1)

Value: = 103.5 degree C
Decomposition: no
Sublimation: no
Method: other
Year: 1978
GLP: no
Remark: high purity sample
Source: Bayer AG Leverkusen
30-APR-1992 (1)

2.2 Boiling Point

Value: >= 200 degree C at 1013 hPa
Decomposition: yes
Method: other
Year: 1976
GLP: no
Remark: DCBS was heated in an open glass vessel under air and normalpressure with a heating rate of 10 degree C per min, and in a closed glass vessel with a heating rate of 5 degree C per min. In both experiments a very strong exothermic decomposition could be observed at temperatures of >= 200 degree C using DTA.
Thermogravimetric analysis showed that when a DCBS sample was kept at a constant temperature of 230 degree C on a balance, after 5 min more than 50 % w/w of the sample were volatilized. After 30 and 45 min approx. 20 % w/w of the sample were still on the balance.
Source: Bayer AG Leverkusen
04-MAY-1992 (1)

2.3 Density

Type: bulk density
Value: ca. 1.2 g/cm3 at 20 degree C
Method: other
Year: 1982
GLP: no
Source: Bayer AG Leverkusen
30-APR-1992 (1)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: ca. .00075 hPa at 120 degree C
Method: other (measured): comparable to OECD Guide-line 104
Year: 1978
GLP: no
Source: Bayer AG Leverkusen
30-APR-1992 (1)

Value: ca. .0035 hPa at 140 degree C
Method: other (measured): comparable to OECD Guide-line 104
Year: 1978
GLP: no
Source: Bayer AG Leverkusen
30-APR-1992 (1)

2.5 Partition Coefficient

log Pow: 5.951 at 25 degree C
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
18-OCT-2001 (2)

log Pow: 4.8
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year:
Source: Bayer AG Leverkusen
04-DEC-1995 (3)

2.6.1 Water Solubility

Value: ca. 30 mg/l at 25 degree C
Qualitative: of very low solubility
Method: other
Year: 1988
GLP: no
Source: Bayer AG Leverkusen
30-APR-1992 (1)

2.6.2 Surface Tension
-

2.7 Flash Point

Value:	ca. 180 degree C
Type:	closed cup
Method:	other: DIN 51758
Year:	1989
GLP:	no
Remark:	The substance being solid, flash point determination according to the EEC-Directive cannot be carried out. The determination was done using a molten sample following method DIN 51758.
Source:	Bayer AG Leverkusen

04-MAY-1992 (1)

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .0000000001138512 cm3/(molecule * sec)
Degradation: 50 % after 1.1 hour(s)
Method: other (calculated): AOP Program (v1.89)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
18-OCT-2001 (2)

3.1.2 Stability in Water

Type: abiotic
Method: other
Year: 1988 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Result: DCBS hydrolyzed slowly at a temperature of 100 degree C, 2-mercaptobenzothiazole (MBT), MBT-sulfonic acid, 2-hydroxybenzothiazole and dicyclohexylamine were identified as decomposition products. Addition of strong bases or acids accelerated the reaction.
Source: Bayer AG Leverkusen
30-APR-1992 (1)

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - water - soil - sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.0457	2.25	1000	2.42e-013
Water	7.15	900	1000	7.39e-015
Soil	39.9	900	1000	8.32e-017

Sediment 52.9 3.6e+003 0 4.97e-015

Persistence Time: 1.45e+003 hr
Reaction Time: 1.65e+003 hr
Advection Time: 1.15e+004 hr
Percent Reacted: 87.5
Percent Advected: 12.5
Reliability: (2) valid with restrictions
Accepted calculation method
18-OCT-2001 (2)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 100 mg/l related to Test substance
Degradation: ca. 2 % after 28 day
Result: under test conditions no biodegradation observed
Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"
Year: 1989 GLP: no
Test substance: other TS: commercial product
Source: Bayer AG Leverkusen
04-DEC-1995 (1)

Type: aerobic
Inoculum: other: Japanese standard activated sludge
Concentration: 100 mg/l related to Test substance
Degradation: 0 % after 28 day
Method: OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year: 1994 GLP: yes
Test substance:
Source: Bayer AG Leverkusen
04-DEC-1995 (4)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: ThOD: 2300 mg/g
Source: Bayer AG Leverkusen
09-DEC-1993 (1)

3.7 Bioaccumulation
-

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: semistatic
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: > 1000
Method: other: OECD Guideline 203
Year: 1981 GLP: no
Test substance: other TS: 99.9 %
Remark: Stock solution was prepared with ethanol with ultrasonication.
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Guideline study
18-OCT-2001 (3) (5)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: 15
Method: other
Year: 1988 GLP: no
Test substance: other TS: commercial product
Remark: The substance was dispersed in water equivalent to a concentration of 1 g/l, stirred for 2 h and subsequently filtered. The filtrate was tested on Brachydanio rerio: no observed effects in the undiluted sample (DOC of the filtrate : 15 mg/l).
Source: Bayer AG Leverkusen
26-JAN-1995 (1)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: > 1000
Method: other: OECD Guideline 202
Year: 1984 GLP: no
Test substance: other TS: 99.9 %
Remark: static
stock solution was prepared with DMSO:HCO-40 = 9:1
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Guideline study
18-OCT-2001 (3)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species:	Selenastrum capricornutum (Algae)
Endpoint:	biomass
Exposure period:	72 hour(s)
Unit:	mg/l Analytical monitoring: no
NOEC:	10
EC50:	16
Method:	other: OECD Guideline 201
Year:	1984 GLP: no
Test substance:	other TS: 99.9 %
Remark:	Stock solution was prepared with DMSO:HCO-40 = 9:1
Source:	Bayer AG Leverkusen
Reliability:	(1) valid without restriction Guideline study

18-OCT-2001 (3) (5)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:	aquatic
Species:	activated sludge
Exposure period:	3 hour(s)
Unit:	mg/l Analytical monitoring: no
EC0:	>= 10000
Method:	ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year:	1988 GLP: no
Test substance:	other TS: commercial product
Remark:	The substance was dispersed in the test medium equivalent to a concentration of 10 g/l.
Source:	Bayer AG Leverkusen

09-DEC-1993 (1)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species:	Daphnia magna (Crustacea)
Endpoint:	reproduction rate
Exposure period:	21 day
Unit:	mg/l Analytical monitoring: no
NOEC:	10
LOEC:	18
EC50:	40
Method:	other: OECD Guideline 202 (1984)
Year:	1994 GLP: no
Test substance:	other TS: 99.9 %
Remark:	21d-EC50 (immobility): 140 mg/l static Stock solution was prepared with DMSO:HCO-40 = 9:1
Source:	Bayer AG Leverkusen

31-MAY-1996 (3) (5)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain:
Sex: male/female
Number of Animals:
Vehicle:
Value:
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: GLP: yes
Test substance: other TS: purity 99.2 %
Remark: Fatal cases were found in males at the doses of more than 2367 mg/kg and in females of more than 1401 mg/kg. But, no dose-related mortalities were observed.
value: > 1,821 mg/kg in male; > 1,077 mg/kg in female
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP Guideline study
18-OCT-2001 (6)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 10000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
20-OCT-1993 (7)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 6420 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
20-OCT-1993 (8)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 8500 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
10-MAY-1994 (9)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Monsanto
Bayer AG Leverkusen
06-JUN-1994 (10)

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 2000 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: purity = 96%
Source: Monsanto
Bayer AG Leverkusen
26-APR-2001 (10)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: s.c.
Value: > 5000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
Test substance: DCBS of technical and analytical grade was tested.
20-OCT-1993 (11)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result:
EC classificat.:
Method:
Year: GLP:
Test substance:
Remark: 20 mg/24h
effect: moderate
Source: Bayer AG Leverkusen
20-OCT-1993 (12)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result:
EC classificat.:
Method: other: exposure time: 24 h (no further data)
Year: GLP:
Test substance:
Remark: effect: practically non-irritating

Source: Bayer AG Leverkusen
26-APR-2001 (10)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method:
Year: GLP:
Test substance:
Remark: 500 mg/24 h
effect: mild
Source: Bayer AG Leverkusen
20-OCT-1993 (12)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method: other: exposure time: 24 h (no further data)
Year: GLP:
Test substance:
Remark: effect: practically non-irritating
Source: Monsanto
Bayer AG Leverkusen
06-JUN-1994 (10)

5.3 Sensitization

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method:
Year: GLP:
Test substance: other TS: Santocure DCBS; purity = 98%
Source: Monsanto
Bayer AG Leverkusen
26-APR-2001 (13)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: 2/135 showed an allergic reaction towards 1 % Cyclohexylbenzothiazyl-sulfenamid
Source: Bayer AG Leverkusen
30-JUL-1998 (14)

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: other: Crj: CD (SD)
Route of admin.: other: oral gavage
Exposure period: males: 44 days including 14 days before mating; females: from 14 days before mating to day 3 of lactation
Frequency of treatment: 7 days/week
Post. obs. period:
Doses: 0, 6, 25, 100, 400 mg/kg (10 animals/group)
Control Group: yes, concurrent vehicle
Method: other: OECD Combined Repeat dose and reproductive/Developmental Screening Toxicity Test
Year: GLP: yes
Test substance: other TS: purity 99.2 %
Result: In the cage side observation, salivation were noted in the 400 mg/kg male group, and decreased locomotor activity were noted in 100 mg/kg or more female groups. At a dose of 400 mg/kg, food consumption decreased prior to the mating and during the pregnancy, and body weight gain decreased at late stage of pregnancy. In urinalysis, increased ketone bodies

were noted in 400 mg/kg males. There are no hematological changes between the treated and control groups of both sexes. Increased relative kidney weights and decreased absolute thymus weights were noted in 400 mg/kg male group and 400 mg/kg both male and female groups, respectively. In histopathological examination, fatty degeneration of the renal tubular epithelia, vacuolation of the adreno-cortical cells and atrophy of the spleen were observed at doses of 100 and 400 mg/kg female groups. Fatty degeneration of liver cells were observed in 400 mg/kg male group, and congestion of liver was noted in 400 mg/kg female group. Also, hyaline droplets in the renal tubular epithelia were observed in 100 and 400 mg/kg male groups.

Source: Bayer AG Leverkusen

Reliability: (1) valid without restriction
GLP Guideline study

18-OCT-2001 (15)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 4 w
Frequency of treatment: daily
Post. obs. period: no data
Doses: 2000, 3000, 5000, 7500 or 10000 ppm (ca. 133, 200, 333, 500 or 667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance: other TS: Santocure DCBS

Result: no significant changes related to treatment were found in hematology or clinical chemistry evaluations, terminal organ weights, or organ/body weight ratios or gross necropsy examinations; dose-related depression in body weight gain and reduced feed consumption on a mg/kg bw/d basis was noted in all treatment groups in comparison to controls

Source: Monsanto
Bayer AG Leverkusen

18-OCT-2001 (16)

Species:	rat	Sex:	male/female
Strain:	Sprague-Dawley		
Route of admin.:	oral feed		
Exposure period:	3 months		
Frequency of treatment:	daily		
Post. obs. period:	no data		
Doses:	2500 or 5000 ppm (ca. 167 or 333 mg/kg bw/d)		
Control Group:	yes		
Method:			
Year:		GLP:	yes
Test substance:	other TS: Santocure DCBS; purity = 96%		
Remark:	species: unspecified, probably rat		
Result:	reduced body weight gain and reduced food consumption in both sexes in both treatment groups were observed; no target organ toxicity or histopathological findings were suggested		
Source:	Monsanto Bayer AG Leverkusen		

18-OCT-2001 (17)

Species:	rat	Sex:	male
Strain:	no data		
Route of admin.:	inhalation		
Exposure period:	15 d		
Frequency of treatment:	2h/d		
Post. obs. period:	no data		
Doses:	340-400 mg/m3		
Control Group:	other: no data		
Method:			
Year:		GLP:	
Test substance:			
Result:	No effect except mucous membrane irritaion were observed. No pronounced liver or kidney changes were observed.		
Source:	Bayer AG Leverkusen		

18-OCT-2001 (9)

5.5 Genetic Toxicity 'in Vitro'

Type: Bacterial reverse mutation assay
System of testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration: 0, 312.5, 625, 1250, 2500, 5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Japanese Guideline for Screening Mutagenicity testing of chemicals
Year: GLP: yes
Test substance: other TS: commercial, purity: 99.5 %
Remark: procedure: plate incorporation method
Result: cytotoxicity conc: with and without metabolic activation: 5000 ug/plate; precipitation conc: 312.5 ug/plate
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Meets National standards method
18-OCT-2001 (18)

Type: Bacterial reverse mutation assay
System of testing: E. coli WP 2 uvrA
Concentration: 0, 312.5, 625, 1250, 2500, 5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Japanese Guideline for Screening Mutagenicity testing of chemicals
Year: GLP: yes
Test substance: other TS: commercial, purity: 99.5 %
Remark: procedure: plate incorporation method
Result: cytotoxicity conc: with and without metabolic activation: 5000 ug/plate, precipitation conc: 312.5 ug/plate
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Meets National standards method
18-OCT-2001 (18)

Type: Cytogenetic assay
System of testing:
Concentration: -S9 (continuous treatment) 0, 0.21, 0.41, 0.82 mg/ml; -S9 (short-term treatment) 0, 0.9, 1.8, 3.5 mg/ml; +S9 (short-term treatment) 0, 0.9, 1.8, 3.5 mg/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result:
Method: other: Japanese Guideline for Screening Mutagenicity testing of chemicals
Year: GLP: yes

Test substance: other TS: commerical, purity: 99.5 %
Result: cytoxtoxicity conc: with and without metabolic activation: > 3.5 mg/ml; genotoxic effects: clastogenicity with and without metabolic activation: negative, polyploid induction: with metabolic activation: negative, without metabolic activation: positive
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Meets National standards method
18-OCT-2001 (18)

Type: Ames test
System of testing: S. typhimurium TA 100, TA 98
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
04-MAY-1992 (19)

Type: Ames test
System of testing: Salmonella typhimurium (no further data)
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP: no data
Test substance:
Source: Monsanto
Bayer AG Leverkusen
26-APR-2001 (20)

Type: HGPRT assay
System of testing: Chinese hamster ovary cells
Concentration: up to 500 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance: other TS: Santocure DCBS; purity = 96%
Source: Monsanto
Bayer AG Leverkusen
26-APR-2001 (21)

Type: Unscheduled DNA synthesis
System of testing: primary rat hepatocytes
Concentration: up to and including 50 ug/ml
Cytotoxic Conc.:
Metabolic activation:
Result: negative
Method:
Year: GLP:
Test substance: other TS: Santocure DCBS
Source: Monsanto
Bayer AG Leverkusen
06-JUN-1994 (22)

5.6 Genetic Toxicity 'in Vivo'

Type: Cytogenetic assay
Species: rat Sex: male/female
Strain: no data
Route of admin.: gavage
Exposure period: single administration
Doses: 1000 mg/kg bw
Result: negative
Method:
Year: GLP: yes
Test substance: other TS: Santocure DCBS; purity = 96%
Result: Santocure DCBS did not produce chromosome damage as measured by significant increases in chromosome aberrations or chromosome number as compared to concurrent controls in the rat bone marrow assay
Source: Monsanto
Bayer AG Leverkusen
26-APR-2001 (23)

5.7 Carcinogenicity

Species:	rat Sex: male/female
Strain:	Wistar
Route of admin.:	s.c.
Exposure period:	413 d
Frequency of treatment:	once a week
Post. obs. period:	entire lifetime
Doses:	1000 mg/kg bw/week, 20000 mg/kg bw (total amount)
Result:	
Control Group:	other: yes
Method:	other
Year:	1975 GLP: no
Test substance:	as prescribed by 1.1 - 1.4
Remark:	20 animals of each sex, technical and analytical grade DCBS was administered.
Result:	No signs of systemic toxicity were reported, there was no difference between the survival of the control group and the dose group, an increased number of sarcomas located at the injection site was observed in all dose groups.
Source:	Bayer AG Leverkusen

30-JUL-1998 (11)

5.8 Toxicity to Reproduction

Type:	other
Species:	rat Sex: male/female
Strain:	other: Crj: CD (SD)
Route of admin.:	other: oral gavage
Exposure Period:	males: 44 days including 14 days before mating, females: from 14 days before mating to day 3 of lactation
Frequency of treatment:	7 days/week
Premating Exposure Period	
male:	14 days
female:	14 days
Duration of test:	
Doses:	0, 6, 25, 100 or 400 mg/kg (10 animals/sex/group)
Control Group:	yes, concurrent vehicle
NOAEL Parental:	100 mg/kg bw
NOAEL F1 Offspr.:	100 mg/kg bw
Method:	other: OECD Combined Repeat dose and reproductive/Development Screening Toxicity Test
Year:	GLP: yes
Test substance:	other TS: purity 99.2 %
Result:	There were no effects indicative of toxicity on male reproductive performance. Toxic effects were revealed in female and pups at doses of 400 mg/kg. There was decreased number of the corpus lutea in accompany of decreases in number of implantation sites and litter size. One dam died during the delivery and another two had prolonged gestation length. All dams lost their litters at delivery or by day 4

of lactation. Therefore, there were decreases in reproduction/development parameters such as gestation index, number of live pups at birth, live birth index and viability index on day 4 of lactation. There were no effects on the mating and fertility, and morphogenesis in pups.

Source: Bayer AG Leverkusen

Reliability: (1) valid without restriction
GLP Guideline study

18-OCT-2001 (15)

5.9 Developmental Toxicity/Teratogenicity

Species: rat Sex: male/female
Strain: other: Crj: CD (SD)
Route of admin.: gavage
Exposure period: males: 44 days including 14 days before mating, females: from 14 days before mating to day 3 of lactation
Frequency of treatment: 7 days/week
Duration of test:
Doses: 0, 6, 25, 100 or 400 mg/kg (10 animals/sex/group)
Control Group: yes, concurrent vehicle
Method: other: OECD Combined Repeat dose and reproductive/Development Screening Toxicity Test
Year: GLP: yes
Test substance: other TS: purity 99.2 %
Result: Toxic effects were revealed in female and pups at doses of 400 mg/kg. There were no effects on the mating and fertility, and morphogenesis in pups.
One dam died during the delivery and another two had prolonged gestation length. All dams lost their litters at delivery or by day 4 of lactation. Therefore, there were decreases in reproduction/development parameters such as gestation index, number of live pups at birth, live birth index and viability index on day 4 of lactation.
Reliability: (1) valid without restriction
GLP Guideline study

18-OCT-2001 (15)

Species: other: chicken Sex:
Strain: no data
Route of admin.: other: see remarks
Exposure period: single administration
Frequency of treatment:
Duration of test: no data
Doses: the highest dose tested was reported to be a saturated acetone solution corresponding to 0.5 umoles per egg (ca. 173 ug)
Control Group: no data specified
Method:
Year: GLP:
Test substance: other TS: Vulkacit DZ
Remark: the test substance was injected into three day chicken embryos
Result: Vulkacit DZ did not produce any evidence of embryotoxic or teratogenic effects
Source: Monsanto
Bayer AG Leverkusen
07-JUN-1994 (24)

5.10 Other Relevant Information

Type: other
Remark: DCBS had no effect on three-day chicken embryos when injected into the air chamber.
Source: Bayer AG Leverkusen
04-MAY-1992 (25) (26)

5.11 Experience with Human Exposure
-

(1) Bayer AG data

(2) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

(3) EA, Japan 'Investigation of the Ecotoxicological Effects of OECD High Production Volume Chemicals'm Office of Healath Studies, Environmental Health Department, Environment Agency, Japan (HPV/SIDS Test conducted by EA, Japan) (1994)

(4) MITI, Japan, Unpublished Report (HPV/SIDS Test conducted by MITI, Japan. Test was performed in CITI, Japan) (1994)

(5) Ueda, S. et al., Fish Acute Toxicity and Algal Growth Inhibition by High Production Volume Chemicals. Nagasaki-ken Eisei Kogai Kenkyushoho 36, 107-110 (1993) (Japanisch !)

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(7) de Groot, A.P., CIVO-TNO, short report

(8) Marhold, J.V., Prehled Prumyslove Toxicol. Org. Latky, pg 1101 (1986), cited in RTECS August 1990

(9) Vorobeva, R.S., Toksikol. Nov. Khim. Veshchestv, Vnedryaemykh Reszin. Shinnuyu Prom. 1968, 89-93, cited in: Chem. Abstr. 71: 20566h

(10) Monsanto Study BD-84-217

(11) Bayer AG data, Report No. 5119, January 1975

(12) Marhold, J.V., Prehled Prumyslove Toxicol. Org. Latky, pg 1101 (1986), cited in RTECS August 1990

(13) Monsanto Study IR-84-230

(14) Heise, H. et al., Dermatrosen 45, 226-228 (1997)

(15) MHW, Japan (1994b): unpublished data cited in SIDS Dossier, August 1995

(16) Monsanto Study BD-87-327

(17) Monsanto Study ML-88-180

(18) MHW, Japan (1994c): unpublished data cited in SIDS Dossier, August 1995

(19) You, X. et al., Huanjing Kexue 3, 39-42 (1982), cited in: Chem. Abstr. 98: 84705t

(20) Monsanto Study HL-84-292

(21) Monsanto Study PK-84-231

(22) Monsanto Study SR-84-291

(23) Monsanto Study HL-84-293

(24) Korhonen, A. et al.: Arch. Environ. Contam. Toxicol. 11, 753-759 (1982)

(25) Korhonen, A. et al., Arch. Environm. Contam. Toxicol. 11, 753-759 (1982)

(26) Korhonen, A. et al., Scand. J. Work Environ. Health 9, 115-119 (1983)

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 95-31-8
CAS No.	95-31-8
EINECS Name	N-tert-butylbenzothiazole-2-sulphenamide
EINECS No.	202-409-1
Molecular Formula	C11H14N2S2

Producer Related Part
- Company: EUROPEAN COMMISSION - European Chemicals Bureau
- Creation date: 11-FEB-2000

Substance Related Part
- Company: EUROPEAN COMMISSION - European Chemicals Bureau
- Creation date: 11-FEB-2000

Memo: Data for RAPA Sulfenamide Accelerators category

Printing date:	12-OCT-2001
Revision date:	11-FEB-2000
Date of last Update:	11-FEB-2000

Number of Pages: 39

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Name: Akzo Nobel Chemicals b.v.
Street: Stationsplein 4, PO Box 247
Town: 3800AE Amersfoort
Country: Netherlands
Phone: +31-33-676767
Telefax: +31-33-676150
Telex: 79322

Name: Bayer Antwerpen N.V.
Street: Haven 507, Scheldelaan 420
Town: Antwerpen
Country: Belgium

Name: BFGoodrich Chemical (Belgie) N.V.
Street: Rue de Verdun/straat 742
Town: 1130 Brussels
Country: Belgium
Phone: 32-2-247-19-11
Telefax: 32-2-247-19-91

Name: GENERAL QUIMICA, S.A.
Street: Km.4 Ctra. de Miranda a Puentelarrá
Town: 01213 LANTARON COMUNION (ALAVA)
Country: Spain
Phone: 947-31 01 45
Telefax: 947-31 38 88
Telex: 39531

Name: Monsanto Europe N.V.
Street: Tervurenlaan, 270-272
Town: 1150 Bruxelles
Country: Belgium

Name: UniroyalChemical Company
Street: Benson Road
Town: 06749 Middlebury, CT
Country: United States
Phone: 203-573-3390
Telefax: 203-573-4531
Telex: 3106710383

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: solid

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

2-Benzothiazolesulfenamide, N-(1,1-dimethylethyl)-
Source: Akzo Nobel Chemicals b.v. Amersfoort
Monsanto Europe N.V. Bruxelles

2-benzothiazolesulfenamide, N-(1,1-dimethylethyl)-
Remark: other: tertiary-butylbenzothiazolesulfenamide
Source: BFGoodrich Chemical (Belgie) N.V. Brussels

Benzothiazolyl-2-tert-butylsulfenamide
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

Benzothiazyl-2-tert-butylsulfenamid
Source: Bayer Antwerpen N.V. Antwerpen

Cure-rite BBTS
Source: UniroyalChemical Company Middlebury, CT

Delac NS
Source: UniroyalChemical Company Middlebury, CT

N-(1,1-dimethylethyl)-2-benzothiazolesulfenamide
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

N-tert.-butyl-2-benzothiazolsulfenamide
Source: Bayer Antwerpen N.V. Antwerpen

N-tert.butyl-2-benzothiazyl sulphenamide
Source: Akzo Nobel Chemicals b.v. Amersfoort

Perkacit NS
Source: UniroyalChemical Company Middlebury, CT

Santocure NS
Source: UniroyalChemical Company Middlebury, CT

TBBS
Source: UniroyalChemical Company Middlebury, CT
Akzo Nobel Chemicals b.v. Amersfoort
Bayer Antwerpen N.V. Antwerpen
Monsanto Europe N.V. Bruxelles

TBBS/EGC
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

tertiary-Butylbenzothiazolesulfenamide
Source: Akzo Nobel Chemicals b.v. Amersfoort
Monsanto Europe N.V. Bruxelles

Vulkacit NZ
Source: UniroyalChemical Company Middlebury, CT
Bayer Antwerpen N.V. Antwerpen

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity

Quantity 10 000 - 50 000 tonnes

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern

Type: type
Category: Use in closed system

Type: type
Category: Use resulting in inclusion into or onto matrix

Type: industrial
Category: Chemical industry: used in synthesis

Type: industrial
Category: Polymers industry

Type: industrial
Category: other: Rubber processing industry

Type: use
Category: Vulcanizing agents

Type: use
Category: other: vulcanisation of natural and sythetic rubber

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values

Type of limit: TLV (US)
Limit value: 10 mg/m3
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

Type of limit:
Limit value:
Remark: Occupational exposure limit has not been set.
Source: Akzo Nobel Chemicals b.v. Amersfoort

1.9 Source of Exposure

Source: UniroyalChemical Company Middlebury, CT

Remark: Method of manufacturing: oxidative coupling of 2-mercaptobenzothiazole and t-butylamine using either sodium hypochlorite or chlorine gas and air.
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution

Classified by:
Labelled by:
Class of danger: 0 (generally not water polluting)
Source: UniroyalChemical Company Middlebury, CT

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks

Remark: Disposal: Controlled combustion.

Transport information:
UN number: NP
ADR/RID: NP
IATA-DGR: NP
IMDG: NP
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value: ca. 103 degree C
Decomposition: no
Sublimation: no
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(1)

Value: = 104 degree C
Method: other: no data
GLP: no data
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

Value: ca. 109 degree C
Decomposition: no
Sublimation: no
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(2)

2.2 Boiling Point

Value:
Source: Monsanto Europe N.V. Bruxelles

2.3 Density

Type: density
Value: ca. 1.28 g/cm3 at 25 degree C
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(2)

Type: density
Value: = 1.29 g/cm3 at 25 degree C
Method: other: no data
GLP: no data
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

Type: density
Value: = 1.29 g/cm3
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(3)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: .000000611 hPa at 20 degree C
Method: other (measured)
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(1)

Value: .00000137 hPa at 25 degree C
Method: other (measured)
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(1)

Value: .0000547 hPa at 25 degree C
Method: other (calculated)
Source: Monsanto Europe N.V. Bruxelles
(1)

2.5 Partition Coefficient

log Pow: 4.38
Method: other (measured)
Year:
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(4)

log Pow: 4.67 at 22.4 degree C
Method:
Year: 1991
GLP: yes
Source: Monsanto Europe N.V. Bruxelles
(1)

2.6.1 Water Solubility

Value: < 1 mg/l at 20 degree C
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(1)

Value: .3 mg/l
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
(5)

Remark: No soluble
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

2.6.2 Surface Tension
-

2.7 Flash Point
-

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation
-

3.1.2 Stability in Water

Type:	abiotic
t1/2 pH7:	= 6.1 hour(s)
Degradation:	= 100 % after 24 hour(s) at pH 7
Method:	other: ABC Laboratories method
Year:	1984 GLP: yes
Test substance:	other TS: Monsanto product 1983.
Result:	Report indicates that Santocure NS hydrolyzed completely. Mercaptobenzothiazole and t-butylamine were identified as hydrolysis products. Half-life should be viewed as an estimate.
Source:	Monsanto Europe N.V. Bruxelles
Test condition:	Deionized water filtered through a 0.45 micron filter and adjusted to pH 7.00 +/- 0.05 using 0.1 M NaOH/0.1 M KH2PO4 buffer system. Stock solutions were prepared in acetone and then aliquots transferred to the water system.
Test substance:	Santocure NS supplied by Monsanto Polymer Products Company November 30, 1983. Sample was from lot number NC06-107 with a purity of 97%.

(6)

Type:	abiotic
t1/2 pH7:	= 10.4 - 13.2 hour(s)
t1/2 pH9:	= 40.5 hour(s)
t1/2 pH 5 :	= 5.1 hour(s)
Method:	other: ABC Laboratories Method (1984).
Year:	1984 GLP: yes
Test substance:	other TS: Monsanto product 1983.
Result:	Test results confirm the results obtained in Monsanto report AB-84-X128. Santocure NS has a hydrolysis half-life less than 24 hours in water. Presence of sunlight did not impact rate of disappearance of Santocure NS. Data suggest that Santocure NS hydrolyzes to yield mercaptobenzothiazole.
Source:	Monsanto Europe N.V. Bruxelles
Test condition:	Deionized and environmental water (well water) were filtered through a 0.45 micron filter. The pH was adjusted to one of 3 pHs. At pH 5 a potassium hydrogen phthalate buffer was used, at pH 7 a potassium dihyrogenphosphate buffer was used while at pH 9 a sodium borate buffer was used. Hydrolysis in sunlight and in the dark and for samples prepared in buffered well water and in buffered deionized water were used to evaluate the impact of sunlight and other minerals on the hydrolysis rate. Neither sunlight nor added minerals from the well water impacted hydrolysis significantly.
Test substance:	Santocure NS supplied by Monsanto Polymer Products Company November 30, 1983. Sample was from lot number NC06-107 with a purity of 97%.

(7)

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments
-

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type:	aerobic
Inoculum:	activated sludge
Concentration:	100 mg/l
Degradation:	0 % after 28 day
Method:	OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year:	1991 GLP: yes
Test substance:	other TS: 99%
Source:	Monsanto Europe N.V. Bruxelles

(8)

Type:	aerobic
Inoculum:	activated sludge, adapted
Concentration:	29.4 mg/l related to Test substance
Result:	other: at 32 days 63.5% of theoretical amount of CO2 had evolved.
Method:	other: Monsanto shake flask procedure.
Year:	1975 GLP: no data
Test substance:	other TS
Source:	Monsanto Europe N.V. Bruxelles
Test condition:	Monsanto shake flask procedure: 60 mL of acclimated bacterial seed is mixed with 440 mL of minimal salts media in fluted 2-liter flask. Appl. Microbiol. 30:922 (1975).
Test substance:	Monsanto Industrial Chemicals MIC 270582.

(9)

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation
-

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type:	flow through
Species:	Pimephales promelas (Fish, fresh water)
Exposure period:	14 day
Unit:	mg/l Analytical monitoring: yes
LC50:	> .3
Method:	other: Monsanto protocol
Year:	1979 GLP: no data
Test substance:	other TS: received from John Vander Kooi
Remark:	TOXICTY ABOVE WATER SOLUBILITY (.3 mg/l); 14day LC50>2.33 mg/l
Source:	Monsanto Europe N.V. Bruxelles
Test condition:	continuous flow diluter; rate=2 ml/l; solvent=dimethylformamide (.33 mg/l); mean weight=.43 gm; mean length=38 mm

(10)

Type:	static
Species:	Brachydanio rerio (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: yes
Method:	other: Directive 67/548/EEC "Acute toxicity to fish" Draft 1992
Year:	1993 GLP: yes
Test substance:	other TS: 99%
Remark:	No mortality beneath the detection limit of the analytical method (0.5 mg/ml)
Source:	Monsanto Europe N.V. Bruxelles

(8)

Type:	static
Species:	Lepomis macrochirus (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: no
LC50:	> .3
Method:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year:	1984 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	TOXICITY ABOVE WATER SOLUBILITY (.3 mg/l); 96hr LC50=1.2 mg/l (C.I.=.98-1.6 mg/l); 24hr LC50=3.6 mg/l; 48hr LC50=1.5 mg/l
Source:	Monsanto Europe N.V. Bruxelles
Test condition:	solvent=acetone; mean length=3.8 cm; 22C

(11)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: > .3
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE WATER SOLUBILITY (.3 mg/l); 96hr LC50=1.6 mg/l (C.I.=1.3-1.9 mg/l); 24 & 48 hr LC50=1.6 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: solvent=acetone; mean length=3.7 cm; 12C

(11)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: > .3
LC50: > .3
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE WATER SOLUBILITY (.3 mg/l); 96 hr LC50=21 mg/l (C.I.=6-27 mg/l); 96h NOEC=5.6 mg/l; 24hr LC50=24 mg/l; 48hr LC50=21 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: solvent=acetone; 22C

(12)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: > .3
EC50: > .3
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE WATER SOLUBILITY (0.3 mg/l); 24hr & 48hr EC50>100 mg/l; 48 hr NOEC=100 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: solvent=acetone

(13)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species:	Selenastrum capricornutum (Algae)
Endpoint:	biomass
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: no
EC50:	> .3
Method:	other: U.S. EPA (1971) Algal Assay Procedure: Bottel Test EPA1972-795-146/1
Year:	1971 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	TOXICITY ABOVE WATER SOLUBILITY (.3 mg/l); 96hr EC50=4 mg/l (C.I.=1-15 mg/l); in vivo chlorophyll results: 24 hr EC50>10 mg/l, 48hr EC50=6 mg/l, 72 & 96hr EC50=4 mg/l
Source:	Monsanto Europe N.V. Bruxelles
Test condition:	solvent=acetone; 24C; 4000 lux, 10,000 cells/ml

(14)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:	aquatic
Species:	activated sludge
Exposure period:	3 hour(s)
Unit:	mg/l Analytical monitoring: no
EC50:	> 10000
Method:	ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year:	1990 GLP: yes
Test substance:	other TS: 99%
Source:	Monsanto Europe N.V. Bruxelles

(8)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	> 6310 mg/kg bw
Method:	other: Younger Laboratory method
Year:	1973 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	TEST CONDITIONS: mode of administration: gavage number of animals: 5/dose (M,F) TEST RESULTS: lung congestion; liver, discoloration; GIT, inflammation; apetite, decr; activity, decr; weakness; collapse.
Source:	Monsanto Europe N.V. Bruxelles

(15)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	= 6850 mg/kg bw
Method:	other
Year:	GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	TEST CONDITIONS: number of animals: 2 M, 3 F vehicle: water (10% w/w suspension) TEST QUALITY: too few animals used TEST RESULTS: mortality
Source:	Monsanto Europe N.V. Bruxelles

(16)

Type: LD0
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 10000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
number of animals: 1 M, screening test
doses: one dose level
vehicle: water (25 % w/w suspension)
TEST RESULTS:
no mortality
Source: Monsanto Europe N.V. Bruxelles
(17)

Type: LDLo
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 7940 mg/kg bw
Method: other: no data
Year: 1990 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)
(18)

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 7940 mg/kg bw
Method: other: Younger Laboratories method
Year: 1973 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
mode of administration: not given
number of animals: 1 M, 1 F

exposure time: 24 hours
vehicle: 40% suspension in corn oil
Source: Monsanto Europe N.V. Bruxelles
(15)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: < 7940 mg/kg bw
Method: other: no data
Year: 1990 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)
(18)

Type: LD0
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 6000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
number of animals: 1 M, 1 F/dose
TEST RESULTS:
all animals survived at 6000 mg/kg bw
Source: Monsanto Europe N.V. Bruxelles
(19)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 5000 mg/kg bw
Method: other: no data
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)
(20)

Type: LC50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 5000 mg/kg bw
Method: other
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(21)

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.v.
Value: = 180 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

(22)

Type: LC50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.v.
Value: = 180 mg/kg bw
Method: other
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(23)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: not irritating
EC classificat.: not irritating
Method: other: Younger Laboratories method
Year: 1973 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
mode of administration: as per FHSA
exposure time: 24 hours
reading times: 24, 48, 72, 168 hours
vehicle: water
skin: intact
number of animals: 6

TEST RESULTS:
EU mean erythema score: 0.0
EU mean edema score: 0.0
PII: 0/8
Source: Monsanto Europe N.V. Bruxelles

(15)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: slightly irritating
EC classificat.: not irritating
Method: other: modified Draize
Year: 1944 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
number of animals: 1 M, 2 F
exposure time: 24 hours
PII: 1.0/8
healing time: 2 hours
Source: Monsanto Europe N.V. Bruxelles

(17)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: slightly irritating
EC classificat.: not irritating
Method: other: modified Draize
Year: 1944 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
number of animals: 6 M
exposure time: 24 hours
skin: intact

TEST RESULTS:
PII: 1.5/8.0
healing time: not cleared in 72 hours
Source: Monsanto Europe N.V. Bruxelles

(24)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals:
Result: slightly irritating
EC classificat.: not irritating
Method: Draize Test
Year: 1944 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
number of animals: 6
TEST RESULTS:
EU mean erythema score: 2.53
EU mean chemosis score: 0
EU mean corneal score: 0
EU mean iritis score: 0
Draize score: 2.5/110
Source: Monsanto Europe N.V. Bruxelles

(15)

Species:	rabbit
Concentration:	
Dose:	
Exposure Time:	
Comment:	
Number of Animals:	
Result:	slightly irritating
EC classificat.:	not irritating
Method:	other: modified Draize
Year:	1944 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	TEST CONDITIONS: number of animals: 2 M, 1 F TEST RESULTS: Draize score: 2.4/110 healing time: 72 hours
Source:	Monsanto Europe N.V. Bruxelles

(17)

Species:	rabbit
Concentration:	
Dose:	
Exposure Time:	
Comment:	
Number of Animals:	
Result:	slightly irritating
EC classificat.:	not irritating
Method:	Draize Test
Year:	1944 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	TEST CONDITIONS: number of animals: 6 M TEST RESULTS: Draize score: 2.5/110.0 healing time: 48 hours
Source:	Monsanto Europe N.V. Bruxelles

(25)

5.3 Sensitization

Type:	Buehler Test
Species:	guinea pig
Number of Animals:	
Vehicle:	
Result:	sensitizing
Classification:	sensitizing
Method:	other: Pharmakon Laboratory method
Year:	1980 GLP: yes
Test substance:	as prescribed by 1.1 - 1.4
Remark:	TEST CONDITIONS: The test material came from three different locations. It was applied in a 25% preparation in ethanol.
Source:	Monsanto Europe N.V. Bruxelles

(26)

Type:	Patch-Test
Species:	human
Number of Animals:	
Vehicle:	
Result:	sensitizing
Classification:	sensitizing
Method:	other
Year:	1969 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	55 subjects (18 M/ 37 F); 24 hour occluded, alternate day patches for 14 days. 9 0f 55 showed sensitization; not a primary irritant
Source:	Monsanto Europe N.V. Bruxelles

(27)

Type:	Patch-Test
Species:	human
Number of Animals:	
Vehicle:	
Result:	sensitizing
Classification:	sensitizing
Method:	other: Not specified
Year:	1983 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	TEST CONDITIONS: 1% Santocure NS in petrolatum. No testing was carried out to determine if trace quantities of MBT were in the preparation. TEST RESULTS: 13 of 14 subjects who had previously been sensitized by MBT also showed sensitivity reactions when exposed to Santocure NS.
Source:	Monsanto Europe N.V. Bruxelles

(28)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result: sensitizing
Classification: sensitizing
Method: other: Product Investigations method
Year: 1982 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
60% preparation in petrolatum.
TEST RESULTS:
13 of 45 subjects responded during challenge.
Source: Monsanto Europe N.V. Bruxelles

(29)

Type: other
Species: rabbit
Number of Animals:
Vehicle:
Result: not sensitizing
Classification: not sensitizing
Method: other: Pharmakon Laboratory method
Year: 1982 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: The studies were comedogenicity assays.
Three separate samples of Santocure NS were tested in concentrations of 0.01, 0.1, or 10% in chloroform (sample #1), 1, 10, or 100% in chloroform (sample #2), and 0.01, 0.1, or 1% in chloroform (sample #3).
Source: Monsanto Europe N.V. Bruxelles

(30)

5.4 Repeated Dose Toxicity

Species:	rat	Sex: male/female
Strain:	Sprague-Dawley	
Route of admin.:	inhalation	
Exposure period:	4 weeks	
Frequency of treatment:	6 hours/day, 5 days/week	
Post. obs. period:	no	
Doses:	0.0, 0.0024, 0.029, and 0.084 mg/l	
Control Group:	yes	
NOAEL:	= .029 mg/l	
Method:	other: Monsanto Laboratory method	
Year:	1978	GLP: yes
Test substance:	as prescribed by 1.1 - 1.4	
Result:	1) 0.0024 mg/l: no effects. 2) 0.029 mg/l: NOAEL; blood, SGOT, incr. 3) 0.084 mg/l: blood, SGOT, incr; body weight, decr; liver, histopath; lymph nodes, histopath.	
Source:	Monsanto Europe N.V. Bruxelles	

(31)

Species:	rat	Sex: male/female
Strain:	Sprague-Dawley	
Route of admin.:	oral feed	
Exposure period:	4 weeks	
Frequency of treatment:	daily	
Post. obs. period:	none	
Doses:	0, 10, 50, 300, 1000, 3000 mg/kg bw/day	
Control Group:	yes	
NOAEL:	1000 mg/kg bw	
LOAEL:	3000 mg/kg bw	
Method:	other	
Year:	1978	GLP: yes
Test substance:	as prescribed by 1.1 - 1.4	
Remark:	TEST CONDITIONS: number of animals: 5 M, 5 F/dose	
Result:	1) 1000 mg/kg bw/d: no effect; NOAEL. 2) 3000 mg/kg bw/d: body weight, decr; food consumption, decr; LOAEL.	
Source:	Monsanto Europe N.V. Bruxelles	

(32)

Species:	rat Sex: male/female
Strain:	Sprague-Dawley
Route of admin.:	gavage
Exposure period:	30 days
Frequency of treatment:	daily
Post. obs. period:	none
Doses:	0, 100, 300, 1000, and 3000 mg/kg bw/d
Control Group:	yes
LOAEL:	= 100 mg/kg bw
Method:	other: Bio/dynamics Laboratory method
Year:	1981 GLP: yes
Test substance:	as prescribed by 1.1 - 1.4
Remark:	All female rats in the 3000 mg/kg bw/d group and 1 male rat in the 3000 mg/kg bw/d group died by day 6. All other 3000 mg/kg bw/day male rats were sacrificed on day 6 in a moribund condition. TEST CONDITIONS: number of animals: 5/sex/group
Result:	1) 100 mg/kg bw/d: LOAEL; heart weight, decr, F. 2) 300 mg/kg bw/d: body weight, decr, M; heart, weight, decr, F; kidney, weight, incr; liver, weight, incr, F. 3) 1000 mg/kg bw/d: body, weight, decr, M; heart, weight, decr; kidney, weight, incr; liver, weight, incr, F. 4) 3000 mg/kg bw/d: mortality.
Source:	Monsanto Europe N.V. Bruxelles

(33)

Species:	rat	Sex: male/female
Strain:	Sprague-Dawley	
Route of admin.:	gavage	
Exposure period:	90 d	
Frequency of treatment:	daily	
Post. obs. period:	no	
Doses:	0, 100, 300, and 1000 mg/kg bw/d	
Control Group:	yes	
NOAEL:	= 100 mg/kg bw	
LOAEL:	= 300 mg/kg bw	
Method:	other: Monsanto Laboratory method	
Year:	1982	GLP: yes
Test substance:	as prescribed by 1.1 - 1.4	
Remark:	TEST CONDITIONS: number of animals: 5/sex/group	
Result:	1) 100 mg/kg bw/d: NOEL, NOAEL; no effects. 2) 300 mg/kg bw/d: LOAEL; body, weight, decr, M. 3) 1000 mg/kg bw/d: body, weight, decr, M; liver, weight, incr, F; kidney, weight, incr, F; serum, cholesterol, incr, F; urine, specific gravity, incr, F.	
Source:	Monsanto Europe N.V. Bruxelles	

(34)

Species:	rat	Sex: male
Strain:	Sprague-Dawley	
Route of admin.:	gavage	
Exposure period:	1-3 days	
Frequency of treatment:	multiple daily doses (varied)	
Post. obs. period:	up to 14 days	
Doses:	up to 40 grams total dose	
Control Group:	no	
NOAEL:	> 40000 mg/kg bw	
Method:	other: screen 1 male/ dose	
Year:		GLP: no data
Test substance:	as prescribed by 1.1 - 1.4	
Remark:	TEST CONDITIONS: number of animals: 1 M/dose doses: ranged from 15 to 40 grams/kg bw.	
Source:	Monsanto Europe N.V. Bruxelles	

(17)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 1-5 days
Frequency of treatment: multiple daily doses
Post. obs. period: up to 14 days
Doses: up to 6000 mg/kg bw/d
Control Group: no
NOAEL: > 6000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
1-2 males or females dosed with multiple daily doses for up to 5 days and up to a total of 60 grams/kg of test material.
TEST RESULTS:
all animals survived
Source: Monsanto Europe N.V. Bruxelles

(25)

Species: rabbit Sex: male/female
Strain: New Zealand white
Route of admin.: dermal
Exposure period: 21 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 0, 125, 500, or 2000 mg/kg bw/d
Control Group: yes
NOAEL: > 2000 mg/kg bw
Method: other: IRDC Laboratory method
Year: 1979 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
number of animals: 10/sex/group
Result: 1) 125 mg/kg bw/d:
skin, irritation, slight.
2) 500 mg/kg bw/d:
skin, irritation, slight.
3) 2000 mg/kg bw/d:
NOAEL;
skin, irritation, slight.
Source: Monsanto Europe N.V. Bruxelles

(35)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium strains TA98, 100, 1535, 1537, 1538
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1975 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(36)

Type: Ames test
System of testing: Salmonella typhimurium strains TA98, 100, 1535, 1537, 1538
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1982 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(37)

Type: Ames test
System of testing: Salmonella typhimurium strains TA98, 100, 1535, 1537, 1538
Concentration: up to 500 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Bionetics method
Year: 1975 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(38)

Type: Ames test
System of testing: Salmonella typhimurium strains TA98, 100, 1535, 1537, 1538
Concentration: up to 5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Bionetics method
Year: 1975 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(39)

Type: Bacterial gene mutation assay
System of testing: Salmonella typhimurium TA 98, 100, 1535, 1537, 1538
Concentration: up to 3000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: no data
Year: GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(40)

Type: DNA damage and repair assay
System of testing: E. coli WP2uvrA-(WU-)
Concentration: up to 1000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: ambiguous
Method: other: Bionetics method
Year: 1956 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(39)

Type: Escherichia coli reverse mutation assay
System of testing: E. coli W3110(polA+), p3078(polA-)
Concentration: up to 1000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Bionetics method
Year: 1971 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(39)

Type: HGPRT assay
System of testing: CHO cells
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1984 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(41)

Type: Mammalian cell gene mutation assay
System of testing: CHO cells
Concentration: up to 10 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Bionetics method
Year: 1961 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(39)

Type: Mammalian cell gene mutation assay
System of testing: BALB/3T3 cells
Concentration: up to 35 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Bionetics method
Year: 1987 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: TEST CONDITIONS:
cytotoxicity was observed at a 46% rate at 35 ug/ml.
Source: Monsanto Europe N.V. Bruxelles

(39)

Type: Mammalian cell gene mutation assay
System of testing:
Concentration: 40 mg/l
Cytotoxic Conc.:
Metabolic activation: with
Result:
Method: other: no data
Year: 1983 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)
(42)

Type: Mammalian cell gene mutation assay
System of testing:
Concentration: 35 mg/l
Cytotoxic Conc.:
Metabolic activation: with
Result:
Method: other: no data
Year: 1983 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)
(42)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration: up to 15 ug/ml without S9 and 60 ug/ml with S9
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method: other: Bionetics method
Year: 1975 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: Negative without S9.
Source: Monsanto Europe N.V. Bruxelles
(39)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration: up to 12.5 ug/ml without S9 and 50 ug/ml with S9
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method: other: Bionetics method
Year: 1975 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: Negative without S9.
Source: Monsanto Europe N.V. Bruxelles

(43)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration: up to 100 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method: other: SRI method
Year: 1978 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: Negative without S9.
Source: Monsanto Europe N.V. Bruxelles

(44)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration: up to 100 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method: other: SRI method
Year: 1978 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(45)

Type: Yeast gene mutation assay
System of testing: S. cerevisiae strain D4
Concentration: up to 500 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Bionetics method
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(38)

5.6 Genetic Toxicity 'in Vivo'
-

5.7 Carcinogenicity
-

5.8 Toxicity to Reproduction
-

5.9 Developmental Toxicity/Teratogenicity

Species: rat Sex: female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: days 6-15 of gestation
Frequency of treatment: daily
Duration of test: no
Doses: 0, 50, 150, and 500 mg/kg bw/d
Control Group: yes
NOAEL Maternalt.: > 500 mg/kg bw
NOAEL Teratogen.: > 500 mg/kg bw
Method: other: IRDC method
Year: 1978 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Result: 1) 50 mg/kg bw/d:
no effects.
2) 150 mg/kg bw/d:
no effects.
3) 500 mg/kg bw/d:
maternal:
NOEL, NOAEL;
offspring:
NOEL, NOAEL;
no effects.
Source: Monsanto Europe N.V. Bruxelles

(46)

Species: other Sex: female
Strain: Leghorn
Route of admin.:
Exposure period:
Frequency of treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: TBBS has been reported to be embryotoxic and teratogenic in chick embryos; however, the relevance of this system to man is questionable.
Source: Monsanto Europe N.V. Bruxelles

(47)

Species: other Sex: female
Strain: Leghorn
Route of admin.:
Exposure period:
Frequency of treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: TBBS has been reported to be embryotoxic and teratogenic in chick embryos; however, the relevance of this system to man is questionable.
Source: Monsanto Europe N.V. Bruxelles

(48)

5.10 Other Relevant Information

-

5.11 Experience with Human Exposure

Remark: There are no reports from manufacturing facilities or the customer base which suggest that the experimental sensitizing potential is a problem in practice.
Source: Monsanto Europe N.V. Bruxelles

(1) Bayer AG Data

(2) Monsanto Product Specification

(3) Safety Data Sheet Bayer AG

(4) Monsanto Study MO-92-9052

(5) Monsanto Study MO 92-9052

(6) Monsanto report AB-84-X128.

(7) Monsanto report AB-84-X133.

(8) Bayer AG data

(9) Monsanto report ES-78-SS28.

(10) Monsanto report ES-79-SS22

(11) Monsanto report BN-76-0173

(12) Monsanto report AB-79-0321

(13) Monsanto report AB-78-0119

(14) Monsanto report BN-78-0364

(15) Monsanto Study No. Y-73-222.

(16) Monsanto study SA-44, April 1954, Scientific Associates Lab.

(17) Monsanto study SA-85, Dec. 1954, Scientific Associates Lab.

(18) RTECS: "Registry of Toxic Effects of Chemical Substances" Acute Toxicity Data (ATDAEI): 1, 104, 1990

(19) Monsanto study SA-85, Dec. 1954 Scientific Associates Lab.

(20) RTECS: "Registry of Toxic Effects of Chemical Substances" International Polymer Science and Technology (IPSTB3): 3, 93, 1976

(21) International Polymer Science Tochnology 3, 93. 1976. Reported in RTECS.

(22) RTECS: "Registry of Toxic Effects of Chemical Substances" U.S. Army Armament Research & Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals. (Aberdeen Proving Ground, MD 21010) NX#02241 (CSLNX)

(23) U. S. Army. No date. U. S. Army Armament Research and Development Command. Chemical Systems Laboratory, NIOSH Exchange Chemicals. NY Nos. 02241, 02243, and 02251. As reported in RTECS.

(24) Monsanto study SA-44, Apr 1954, Scientific Associates Lab.

(25) Monsanto study SA-44, Apr. 1954, Scientific Associates Lab.

(26) Monsanto Study Nos. PK-82-41 & 47.

(27) Monsanto study SH-69-10; Food and Drug Research Lab.

(28) Foussereau, J., Menezes-Brandao, F., Cavelier, C., and Herve-Bazin, B. 1983. Allergy to MBT and its derivatives. Contact Dermatitis 9, 514-516.

(29) Monsanto Study No. SH-82-11.

(30) Monsanto Study Nos. PK-82-42 & 48.

(31) Monsanto Study No. IR-78-95.

(32) Monsanto study IR-78-195

(33) Monsanto Study No. BD-81-330.

(34) Monsanto Study No. ML-82-253.

(35) Monsanto Study No. IR-79-263.

(36) Hinderer, R. K., Myhr, B., Jagnnath, D. R., Galloway, S. M., Mann, S. W., Riddle, J. C., and Brusick, D. J. 1983. Mutagenic evaluations of four rubber accelerators in a battery of in vitro mutagenic assays. Environ. Mutagen. 5, 193-215.

(37) You, X., Zhou, Y., and Hu, Y. 1982. Mutagenicity of fourteen rubber accelerators. Huanjing Kexue 3, 39-42 (as reported in Chem. Abstr. 98:84705t).

(38) Monsanto Study No. BO-76-181.

(39) Monsanto Study No. XX-87-9007 (B. F. Goodrich report).

(40) Sumitomo Chemical Co. data, September 24, 1981 (reported to Bayer AG)

(41) B. F. Goodrich. 1984. Evaluation of TBBS (BBTS) in the CHO/HGPRT assay.

(42) RTECS: "Registry of Toxic Effects of Chemical Substances" Environmental Mutagenesis (ENMUDM): 5, 193, 1983

(43) Monsanto Study No. BO-78-222.

(44) Monsanto Study No. SR-81-46.

(45) Monsanto Study No. SR-81-47.

(46) Monsanto Study No. IR-78-101.

(47) Korhonen, A., Hemminki, K., and Vaino, H. 1982. Embryotoxicity of benzothiazoles, benzenesulfohydrazine and dithiodimorpholine to the chicken embryo. Arch. Environ. Contam. Toxicol. 11, 753-759.

(48) Korhonen, A., Hemminki, K., and Vaino, H. 1983. Toxicity of rubber chemicals toward three-day chicken embryos. Scand. J. Work Environ. Health 9, 115-119.

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 95-33-0
CAS No.	95-33-0
EINECS Name	N-cyclohexylbenzothiazole-2-sulphenamide
EINECS No.	202-411-2
TSCA Name	2-Benzothiazolesulfenamide, N-cyclohexyl-
Molecular Formula	C13H16N2S2

Producer Related Part	
Company:	
Creation date:	10-JAN-2000

Substance Related Part	
Company:	
Creation date:	10-JAN-2000

Memo:	Data for RAPA Sulfenamide Accelerators category

Printing date:	17-OCT-2001
Revision date:	
Date of last Update:	17-OCT-2001

Number of Pages:	45

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information
-

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: solid
Purity: >= 96 % w/w
Remark: cooperating companies:
Bayer Antwerpen N.V., Belgium
AKZO Chemicals, Netherlands
Manufacture Landaise de Produits Chimiques, France
Monsanto Europe N.V., Belgium
Uniroyal Chemical Limited, United Kingdom
Source: Bayer AG Leverkusen
27-MAY-1994

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

CBS
03-JUN-1994

N-CYCLOHEXYL-2-BENZOTHIAZOLESULFENAMIDE
03-APR-1992

Santocure accelerator
15-OCT-2001

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern

Type: type
Category: Use resulting in inclusion into or onto matrix
15-OCT-2001

Type: industrial
Category: Polymers industry
Source: Bayer AG Leverkusen
26-APR-1994

Type: use
Category: Vulcanizing agents
Source: Bayer AG Leverkusen
26-APR-1994

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value: 93 - 100 degree C
Decomposition: no
Sublimation: no
Method: other: Handbook value
GLP: no
Testsubstance: other TS: purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

Value: < 96 degree C
Source: Bayer AG Leverkusen
22-SEP-2000 (2)

2.2 Boiling Point

Value:
Decomposition: yes
Remark: n.a., product decomposes during destillation
Source: Bayer AG Leverkusen
18-APR-2001

2.3 Density

Type: density
Value: 1.27 g/cm3 at 25 degree C
Method: other: Handbook value
Testsubstance: other TS: purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

Type: relative density
Value: 1.3 g/cm3 at 25 degree C
Source: Bayer AG Leverkusen
22-SEP-2000 (2)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: < .0000004 hPa at 25 degree C
Method: other (measured)
Reliability: (2) valid with restrictions
22-SEP-2000 (3)

Value: .000000015 hPa at 20 degree C
Source: Bayer AG Leverkusen
16-SEP-1993 (2)

Value: .000000038 hPa at 25 degree C
Source: Bayer AG Leverkusen
16-SEP-1993 (2)

2.5 Partition Coefficient

log Pow: 3.47
Method: other (calculated)
Year:
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (4)

log Pow: 4.93
Method: other (measured)
Year:
Reliability: (2) valid with restrictions
15-OCT-2001 (3)

2.6.1 Water Solubility

Value: .24 other: ppm at 21 degree C
Qualitative: not soluble
pH: 5
Source: Bayer AG Leverkusen
18-APR-2001 (5) (6)

Value: .32 other: ppm at 21 degree C
Qualitative: not soluble
pH: 7
Source: Bayer AG Leverkusen
18-APR-2001 (5) (6)

Value: .48 other: ppm at 21 degree C
Qualitative: not soluble
pH: 9
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
18-APR-2001 (5) (6)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: 168 degree C
Type: closed cup
Method: other: DIN 51758
Year:
Source: Bayer AG Leverkusen
16-SEP-1993 (2)

Value: 176.7 degree C
Type: open cup
Method: other: Cleveland Open Cup
Year:
26-SEP-2000 (7)

2.8 Auto Flammability

Value: 348.9 degree C
26-SEP-2000 (7)

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .00000000007949 cm3/(molecule * sec)
Degradation: 50 % after 1.6 hour(s)
Method: other (calculated): AOP Program vers1.89
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (4)

Type: water
Light source: Xenon lamp
DIRECT PHOTOLYSIS
Halflife t1/2: 26 minute(s)
Method:
Year: GLP:
Test substance:
Remark: light T1/2=26 minutes; Dark control T1/2=9.6 hours
Reliability: (2) valid with restrictions
15-OCT-2001 (3)

3.1.2 Stability in Water

Type: abiotic
Degradation: = 100 % after 24.9 hour(s)
at pH 7 and 20 degree C
Deg. Product: yes
Method: other: ABC Laboratory protocol; see TC
Year: 1984 GLP: yes
Test substance: other TS: purity = 97%
Remark: product = benzothiazole
Source: Monsanto
Bayer AG Leverkusen
Test condition: Buffered deionized water; no light; initial concentration = 1 mg/l
Reliability: (1) valid without restriction
GLP study; Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
15-OCT-2001 (8)

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - biota - sediment(s) - soil - water
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.00923	3.23	1000	2.33e-013
Water	20.7	900	1000	7.78e-015
Soil	78.3	900	1000	1.12e-014
Sediment	0.924	3.6e+003	0	5.78e-015

Persistence Time: 1.01e+003 hr
Reaction Time: 1.27e+003 hr
Advection Time: 4.8e+003 hr
Percent Reacted: 79
Percent Advected: 21

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (4)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 100 mg/l
Degradation: 0 % after 28 day
Result: under test conditions no biodegradation observed
Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"
Year: 1988 GLP: no
Test substance:
Remark: related to O2-consumption
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Meets National standards method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (2)

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 20 mg/l related to Test substance
Degradation: ca. 0 % after 35 day
Result: under test conditions no biodegradation observed
Method: other: Method similar to ASTM draft method no. 2 ASTM Committee E35.24.
Year: 1979 GLP: no data
Test substance:
Remark: Method is similar in principle to Sturm test measuring ultimate biodegradation as CO2 evolved
Source: Monsanto
Bayer AG Leverkusen
15-DEC-1995 (9)

Type: aerobic
Inoculum:
Degradation: 4 %
Method:
Year: GLP:
Test substance: other TS: purity = 97%
27-SEP-2000 (10)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: ThOD: 2070 mg/g
Source: Bayer AG Leverkusen
05-OCT-1993 (2)

3.7 Bioaccumulation
-

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: >= 1000
Method: other: Letale Wirkung beim Zebrabaerbling, UBA-Verfahrensvorschlag, Mai 1984, Letale Wirkung beim Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h
Year: 1989 GLP: no
Test substance:
Remark: direct weight
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
15-OCT-2001 (2)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: > 1000
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 GLP: yes
Test substance: other TS: purity = 97%
Remark: 24, 48, 96hr LC50 >1000 mg/l; water solubility=40 mg/l
Source: Monsanto
Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
15-OCT-2001 (11)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: = 7.9
Method: other: Bionomics Lab protocol; see test conditions
Year: 1976 GLP: no data
Test substance:
Remark: C.I. for LC50=6.9-9.1 mg/l; 24 and 48hr LC50=8.8 mg/l
Source: Monsanto
Bayer AG Leverkusen
Test condition: Carrier-acetone; 22C; length=3.8cm; 15 L water; not fed; no aeration
15-OCT-2001 (12)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: = 5.4
Method: other: Bionomics Lab protocol; see test conditions
Year: 1976 GLP: no data
Test substance: other TS: purity 97%
Remark: C.I. for ELC50=4.5-6.5; 24hr LC50>7.5<10 mg/l; 48hr LC50= 7.5 mg/l
Source: Monsanto
Bayer AG Leverkusen
Test condition: Carrier-acetone; 15 L water; 10 fish/treatment; length= 2.7 cm; no feed; no aeration; 12 C
15-OCT-2001 (12)

Type: flow through
Species:
Exposure period: 14 day
Unit: mg/l Analytical monitoring: yes
Method: other: Springborn Lab protocol; see TC
Year: 1983 GLP: no data
Test substance:
Remark: 20 % mortality at 1.0 mg/l conc. (highest tested conc.)
Source: Monsanto
Bayer AG Leverkusen
Test condition: Nount-Brungs diluter; 19L aquaria; 10 fish/rep.; flow rate=5 tanks volume/day; carrier-acetone; water solubility < 0.48 mg/l; two highest concentration above water solubility
15-DEC-1995 (13)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: Analytical monitoring: yes
Method: other: Letale Wirkung beim Zebrabaerbling, UBA-Verfahrensvorschlag, Mai 1984, Letale Wirkung beim Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h
Year: 1988 GLP: no
Test substance:
Remark: Analytical monitoring: DOC
Die Substanz wurde in der Konzentration 1000 mg/l 2h eluiert, abfiltriert und das Filtrat getestet.
Keine Schadwirkung im Original.
DOC des Filtrats: 12 mg/l
Reliability: 2
Source: Bayer AG Leverkusen
27-SEP-2000 (2)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:		
Species:	Daphnia magna (Crustacea)	
Exposure period:	48 hour(s)	
Unit:	mg/l	Analytical monitoring: no
NOEC:	= 5.6	
EC50:	= 18	
Method:	OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"	
Year:	1984	GLP: yes
Test substance:		
Remark:	C.I. for EC50=14-23 mg/l; 24hr EC50=21 mg/l	
Source:	Monsanto Bayer AG Leverkusen	
Reliability:	(1) valid without restriction GLP guideline study	
Flag:	Critical study for SIDS endpoint	

15-OCT-2001 (14)

Type:		
Species:	Daphnia magna (Crustacea)	
Exposure period:	96 hour(s)	
Unit:	mg/l	Analytical monitoring: no
EC50:	18	
Method:		
Year:		GLP: no data
Test substance:	other TS: purity = 97%	

27-SEP-2000 (15)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species:	Selenastrum capricornutum (Algae)	
Endpoint:	biomass	
Exposure period:	96 hour(s)	
Unit:	mg/l	Analytical monitoring: no
EC50:	= .9 - 1.1	
Method:	OECD Guide-line 201 "Algae, Growth Inhibition Test"	
Year:	1984	GLP: yes
Test substance:	other TS: purity = 97%	
Remark:	C.I. = 0.3-3.2 mg/l; in vivo chlorophyll: 24hr EC50= 3.2 mg/l, 48hr EC50=2.4 mg/l, 72hr EC50=1.2, 96hr EC50= 1.1 mg/l	
Source:	Monsanto Bayer AG Leverkusen	
Test condition:	initial cell inoculum=20X3 cell/ml; 24C; 3800 lux; carrier-DMF	
Reliability:	(1) valid without restriction GLP guideline study	
Flag:	Critical study for SIDS endpoint	

15-OCT-2001 (16)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:	aquatic	
Species:	activated sludge	
Exposure period:	3 hour(s)	
Unit:	mg/l	Analytical monitoring: no
EC50:	> 10000	
Method:	other: Test for Inhibition of Oxygen Consumption by Activated Sludge, ISO 8192	
Year:	1988	GLP: no
Test substance:		
Remark:	direct weight Reliability: 1	
Source:	Bayer AG Leverkusen	

18-DEC-1995 (2)

Type:	soil	
Species:		
Exposure period:	96 hour(s)	
Unit:		Analytical monitoring:
LC50 :		
Method:		
Year:		GLP:
Test substance:		
Remark:	test result: 25 %, when incorporated into nutrient agar, moderately toxic	
Source:	Monsanto Bayer AG Leverkusen	

15-DEC-1995 (17)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type:	LD50
Species:	rat
Strain:	
Sex:	male/female
Number of Animals:	5
Vehicle:	other: corn oil
Value:	= 5300 mg/kg bw
Method:	other
Year:	1973 GLP: no
Test substance:	other TS: purity = 97%
Remark:	test conditions: mode of administration: gavage vehicle: corn oil number of animals: 5 per dose levels (2M, 3F, or 3M, 2F)
Result:	Dercreased appetite and activity; weakness, tremors, collapse, lung: hyperemia; liver: hyperemia; gastro-intestinal tract: inflammation
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag:	Critical study for SIDS endpoint

15-OCT-2001 (18) (19)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	> 5000 mg/kg bw
Method:	other: no data
Year:	1977 GLP: no
Test substance:	other TS: Soxinol CZ
Remark:	1000 mg/kg: No mortality and no toxic symptoms 2500 and 5000 mg/kg: 2/10 males and 3/10 females died 1-3 days after treatment with 5000 mg/kg. After 2-3 hours after administration, irregular respiration, dyspnea, hypersensitivity and ataxia were observed.
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag:	Critical study for SIDS endpoint

15-OCT-2001 (20)

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 8000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: Soxinol CZ-G
Remark: mortality: 0/8; only males
Reliability: (2) valid with restrictions
data are generally regarded as sufficient
Flag: Critical study for SIDS endpoint
15-OCT-2001 (21)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 6850 mg/kg bw
Method: other
Year: GLP: no
Test substance: other TS: purity 96 to 98 %
Reliability: (3) invalid
Reliability: 3
Remark: International Protocol Compliance: No
15-OCT-2001 (22)

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 4000 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: other TS: no data
Reliability: (4) not assignable
Reliability: 4
Remark: the test method is not stated
15-OCT-2001 (23)

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rabbit
Strain:	
Sex:	
Number of Animals:	
Vehicle:	other: corn oil
Value:	> 7940 mg/kg bw
Method:	other
Year:	1973 GLP: no
Test substance:	other TS: purity = 97%
Remark:	mortality: 0/3 test conditions: vehicle: corn oil (40 % suspension of test substance) exposure time: 24 h
Result:	no local effects noted; systemic: decreased appetite and activity
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag:	Critical study for SIDS endpoint

15-OCT-2001 (24) (19)

5.1.4 Acute Toxicity, other Routes

Type:	LD50
Species:	mouse
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Route of admin.:	i.p.
Value:	> 2500 mg/kg bw
Method:	other
Year:	GLP: no
Test substance:	other TS: no data
Reliability:	(2) valid with restrictions Remark: data are generally regarded as sufficient

24-APR-2001 (25)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.v.
Value: 32 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: other TS: no data
Reliability: (4) not assignable
Reliability: 4
Remark: data are derived from papers citing other papers
24-APR-2001 (26)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: other: no data
Value: > 8000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: highest purity available in gum arabic
Reliability: (3) invalid
Reliability: 3
Remark: documentation is not sufficient for an assessment
24-APR-2001 (27)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: slightly irritating
EC classificat.: not irritating
Method: other: Younger Laboratories, St Louis
Year: 1973 GLP: no data
Test substance: other TS: purity = 97%
Result: test result:
EU mean erythema score: 0.00
EU mean edema score: 0.00

PII: 0.00
other effects: none
healing time: not applicable
Test condition: test conditions:
mode of administration: not reported
exposure time: 24 hours
number of animals: 6
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
15-OCT-2001 (18)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: slightly irritating
EC classificat.:
Method: other: Draize-Test
Year: GLP: yes
Test substance: other TS: as prescribed by chapter 1 in dataset of Monsanto
Result: test results:
EU mean erythema score: 0.17
EU mean edema score: 0.00
PII: 0.4/8
other effects: none
healing time: 72 h
Test condition: test conditions:
mode of administration: occlusive
exposure time: 24 h
number of animals: 6
skin: intact and abraded
observation times: 24 h, 72 h
Reliability: (3) invalid
15-OCT-2001 (28) (19)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: no data
Year: GLP: no data
Test substance: other TS: no data
Reliability: (4) not assignable
Reliability: 4
Remark: the test method is not stated

15-OCT-2001 (23)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result:
EC classificat.:
Method: other: no data
Year: GLP: no
Test substance: other TS: no data
Result: effect: no irritation
Reliability: (4) not assignable
Reliability: 4
Remark: the test method is not stated in detail
15-OCT-2001 (23)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals: 6
Result: slightly irritating
EC classificat.: not irritating
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1982 GLP: no
Test substance: other TS: purity = 97%
Result: test results:
EU mean erythema score: 1.7
EU mean chemosis score: 1.1
EU mean corneal opacity score: 0.0
EU mean iritis score: 0.0
Draize score: 1.8/110
other effects: discharge at 1 h and 24 h
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
15-OCT-2001 (18) (19)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method: other: 5 mg/animal
Year: GLP: no
Test substance: other TS: no data
Reliability: (4) not assignable
Reliability: 4
Remark: the test method is not stated in detail
24-APR-2001 (23)

5.3 Sensitization

Type: Buehler Test
Species: guinea pig
Concentration: Induction 25 % open epicutaneous
Number of Animals:
Vehicle:
Result: not sensitizing
Classification: not sensitizing
Method: other: see remarks
Year: GLP: yes
Test substance: other TS: Santocure accelerator
Method: induction exposure: a 25 % concentration of the test material (in ethanol) was applied to the shaved skin of the test animals for 6 hours, once a week, for 3 consecutive weeks; challenge exposure: the test material was administered two weeks after the weekly applications were concluded
Reliability: (1) valid without restriction
Remark: International Protocol Compliance: Yes
15-OCT-2001 (29)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: 1 % in petrolatum
Result: 34/686 patients had a positive patch test result with CBS
Reliability: (2) valid with restrictions
Remark: acceptable, well documented publication
24-APR-2001 (30)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: 1 % in petrolatum
Result: 2/5 patients with contact dermatitis from rubber footwear had a positive patch test result with CBS among others
Reliability: (2) valid with restrictions
acceptable, well documented publication
24-APR-2001 (31)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: 1 % in petrolatum
Result: 11/46 patients with occupational rubber dermatitis had a positive patch test result with CBS
Reliability: (2) valid with restrictions
acceptable, well documented publication
24-APR-2001 (32)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: 1 % in petrolatum
Result: 1/15 thiuram-sensitized patients had a positve patch test result with CBS
Reliability: (2) valid with restrictions
acceptable, well documented publication
24-APR-2001 (33)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other: L. Schwartz and S. Peck, Public Health Reports, 59(17), reprint 2552 (1944)
Year: 1944 GLP: no
Test substance: other TS: as prescribed by chapter 1 in dataset of Monsanto
Method: test conditions:
mode of application: occlusive, patch of 1.5 cm sq on upper arm
exposure time: 24 hours for each exposure
challenge: 10 days after first exposure
observation times: 24 and 48 hours after patch removal
number of volunteers: 204 (94 F, 110 M), age ranging from 15 to 70 years
Result: test results:
no positive reactions after first and second exposure
Reliability: (2) valid with restrictions
24-APR-2001 (34)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other: L. Schwartz and S. Peck, Public Health Reports, 59(17), reprint 2552 (1944)
Year: 1944 GLP: no
Test substance: other TS: as prescribed by chapter 1 in dataset of Monsanto
Result: test result:
no positive reactions on first and second exposure
Test condition: test conditions:
mode of administration: semi-occlusive(?), 1 inch sq patch on upper arm
exposure time: 48 hours
observation times: 24, 48 and 72 hours after patch removal
challenge: 10 days after first exposure
vehicle: none
volunteers: 196 (100 M, 96 F), age ranging from 15 to 70 years
Reliability: (2) valid with restrictions
24-APR-2001 (35)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other: Modified Shelanski
Year: GLP: no
Test substance: other TS: as prescribed by chapter 1 in dataset of Monsanto
Method: test conditions:
number of volunteers: 51, selected from local population
mode of application: 0.2 g of material tested as a 70 % suspension in petrolatum was applied on the webril pad of a Parke-Davis Readi-bandage, the patch was then applied on the skin (occlusive dressing)
induction: series of 12 applications of 24 h duration each carried during weeks 1, 2 and 3.
challenge: a series of 4 applications on virgin sites at week 6
Result: test results:
material acted as a sensitizer in 5 out of 51 volunteers
Reliability: (2) valid with restrictions
24-APR-2001 (36) (37)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS: no data
Remark: Some patch tests carried out with the substance on people suffering from contact dermatitis were positive
Reliability: (2) valid with restrictions
Remark: acceptable, well documented publication:
Bajaj, Foussereau, Rudzki
data are generally regarded as sufficient:
Kantoh, van Dijk, Holness
data are used as supporting evidence:
Eriksson, Heise
24-APR-2001 (38) (39) (40) (41) (42) (43) (44) (45)

Type:	Patch-Test
Species:	human
Number of Animals:	
Vehicle:	
Result:	
Classification:	
Method:	
Year:	GLP: no data
Test substance:	other TS: no data
Remark:	One contact dermatitis patient had a negative patch test result with CBS.
Reliability:	(2) valid with restrictions Remark: acceptable, well documented publication

24-APR-2001 (46)

Type:	other
Species:	human
Number of Animals:	
Vehicle:	
Result:	
Classification:	
Method:	
Year:	GLP:
Test substance:	other TS: CBS
Result:	There are numerous reports in the literature of skin sensitization to CBS; however, in most cases the patients showed positive reactions to other constituents of the "mercapto mix" used for skin testing (MBT, MBTS and MDR)
Reliability:	(4) not assignable Remark: the data quality and test result cannot be evaluated

24-APR-2001 (47) (48) (49) (50) (51) (52)

Type:	other: closed epicutaneous test
Species:	guinea pig
Number of Animals:	
Vehicle:	
Result:	not sensitizing
Classification:	
Method:	other: induction: 0,5 M (50 mg), challenge: 0,5 M or 0,05 M
Year:	GLP: no data
Test substance:	other TS: no data
Reliability:	(2) valid with restrictions Remark: data are generally regarded as sufficient

24-APR-2001 (43)

5.4 Repeated Dose Toxicity

Species:	rat	Sex: male/female
Strain:	no data	
Route of admin.:	oral feed	
Exposure period:	4 w	
Frequency of treatment:	daily	
Post. obs. period:	no data	
Doses:	100, 250, 500, 1000 or 3000 mg/kg bw/d	
Control Group:	yes	
NOAEL:	= 250 mg/kg bw	
Method:		
Year:		GLP: yes
Test substance:	other TS: Santocure accelerator	
Result:	evidence of toxicity, as indicated by reduced body weight gains and food consumption, was noted at the 500, 1000, and 3000 mg/kg bw/d exposure levels	
Reliability:	(2) valid with restrictions Remark: No hematology, no blood biochemistry, no histopathology	
Flag:	Critical study for SIDS endpoint	

15-OCT-2001 (53)

Species:	rat	Sex: no data
Strain:	no data	
Route of admin.:	inhalation	
Exposure period:	4 w	
Frequency of treatment:	6 h/d, 5 d/w	
Post. obs. period:	no data	
Doses:	0.0043, 0.0144 or 0.048 mg/l	
Control Group:	yes	
NOAEL:	= .0144 mg/l	
Method:		
Year:		GLP: yes
Test substance:	other TS: Santocure accelerator	
Result:	elevated clinical chemistry (SGOT) values were observed in mid- and high-exposure animals; microscopic lesions in the conjunctiva, lymph nodes and spleen were noted for high-exposure group animals at an incidence greater than control animals	
Reliability:	(1) valid without restriction International Protocol Compliance: Yes	
Flag:	Critical study for SIDS endpoint	

15-OCT-2001 (54)

Species: rabbit Sex: no data
Strain: no data
Route of admin.: dermal
Exposure period: 21 d
Frequency of treatment: daily
Post. obs. period: no data
Doses: 125, 500 or 2000 mg/kg bw/d
Control Group: yes
Method:
Year: GLP: yes
Test substance: other TS: Santocure accelerator
Result: no evidence of toxicity related to test material administration
Reliability: (1) valid without restriction
International Protocol Compliance: Yes
Flag: Critical study for SIDS endpoint
15-OCT-2001 (55)

Species: rat Sex: no data
Strain: no data
Route of admin.: inhalation
Exposure period: 15 days
Frequency of treatment: 24h/day, daily
Post. obs. period: no
Doses: 300-400 mg/m3
Control Group: no data specified
Method:
Year: GLP: no data
Test substance: other TS: no data
Result: body weight gain unchanged, in few animals slight transient changes in the functional state of the nervous system
Reliability: (4) not assignable
Remark: the test method is not stated in detail
24-APR-2001 (23)

Species: rat Sex: no data
Strain: no data
Route of admin.: gavage
Exposure period: 24 d during a period of 5 w
Frequency of treatment: daily
Post. obs. period: no data
Doses: 0.5 or 1.25 mg/kg bw/d
Control Group: yes
Method:
Year: GLP: no
Test substance: other TS: Santocure accelerator
Result: two females in the high-dose group and one female in the low-dose group died during the experiment; a decrease in body weight gain in the treated animals and an increase in relative thyroid weights were observed; no pathologic changes attributable to treatment were noted
Reliability: (3) invalid
International protocol compliance: no
24-APR-2001 (22)

Species: rat Sex: male/female
Strain: other: H.L.A.
Route of admin.: oral unspecified
Exposure period: 5w
Frequency of treatment: 5d/w, daily
Post. obs. period: 4d
Doses: 500 or 1250 mg/kg bw
Control Group: other: yes
Method: other
Year: GLP: no
Test substance: other TS: purity 96 to 98 %
Result: 1250 mg/kg (females): increased mortality, hyperirritability, sanguineous discharge from the mouth and nostrils; females of both dose groups: changes of the thyroid weight, without pathologic changes (microscopic examination)
Reliability: (3) invalid
International protocol compliance: no
24-APR-2001 (22)

Species:	mouse	Sex: male/female	
Strain:	other: ddy/Slc		
Route of admin.:	oral feed		
Exposure period:	3 months		
Frequency of treatment:	daily		
Post. obs. period:	no		
Doses:	0, 0.04, 0.2, 1.0 %		
Control Group:	yes, concurrent no treatment		
Method:	other		
Year:		GLP: no data	
Test substance:	other TS: Soxinol CZ-G		
Remark:	English Translation of an Informal Japanese report with figures and tables		
Result:	no mortality is reported; reduced body weight gain (1%-dose group); no dose despended changes of hematological/ biochemical parameters and organ weights; no histopathological examinations reported		
Reliability:	(3) invalid Remark: documentation is not sufficient for an assessment		
24-APR-2001			(21)

Species:	rabbit	Sex: no data	
Strain:	no data		
Route of admin.:	oral unspecified		
Exposure period:	3,5 months		
Frequency of treatment:	every second day for the first 1,5 months followed by daily dosing		
Post. obs. period:	no		
Doses:	20 mg/kg bw		
Control Group:	other: yes		
Method:			
Year:		GLP:	
Test substance:			
Result:	no particular symptoms		
Reliability:	(4) not assignable Remark: the test method is not stated in detail		
24-APR-2001			(23)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: no data
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other:
Year: GLP: no
Test substance: other TS: Santocure accelerator
Reliability: (2) valid with restrictions
Remark: International Protocol Compliance: +/- Yes
Flag: Critical study for SIDS endpoint
17-OCT-2001 (56)

Type: Mouse lymphoma assay
System of testing: L5178Y mouse lymphoma assay
Concentration: 0.078 ug/ml to 40 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Litton Bionetics method
Year: 1979 GLP: no
Test substance: other TS: purity = 97%
Remark: test conditions:
solubility in medium: precipitation at 78 ug/ml and higher
cytotoxicity:
-S9:
no survivors at 39 ug/ml, 5.7% to 13.3% relative growth for the concentration range from 15 to 30 ug/ml
+S9:
no survivors at 80 ug/ml, 75.2% relative growth at 40 ug/ml, toxicity was moderate to high in 0.313 to 20 ug/ml concentration range
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
15-OCT-2001 (57)

Type: Ames test
System of testing: Salmonella typhimurium, TA 1535, TA 1537, TA 1538, TA 98, TA 100
Concentration: 0.1 - 500 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: no data
Year: GLP: no
Test substance: other TS: no data
Reliability: (3) invalid
Remark: data are derived from reviews
15-OCT-2001 (58)

Type: Ames test
System of testing: no data
Concentration: no data
Cytotoxic Conc.:
Metabolic activation: no data
Result: negative
Method: other: no data
Year: GLP: no data
Test substance: other TS: no data
Reliability: (4) not assignable
Remark: data are derived from papers citing other papers see Rannug et al. (1984)
24-APR-2001 (59)

Type: Ames test
System of testing: TA 100, TA 98
Concentration: no data
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: no data
Year: GLP: no data
Test substance: other TS: no data
Reliability: (4) not assignable
Remark: data are derived form abstracts
24-APR-2001 (60)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 10-3000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: no data
Year: 1981 GLP: no data
Test substance: other TS: Soxinol CZ
Reliability: (4) not assignable
Remark: the data quality and test result cannot be evaluated
24-APR-2001 (61)

Type: Ames test
System of testing: Salmonella typhimurium, TA 1535, TA 1537, TA 1538, TA 98, TA 100
Concentration: 0 - 150 ug/plate (-S9); 0 - 200 ug/plate (+S9)
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: no data
Year: GLP: no data
Test substance: other TS: technical purity
Reliability: (2) valid with restrictions
Remark: acceptable, well documented publication
24-APR-2001 (62)

Type: Yeast gene mutation assay
System of testing: Saccharomyces cerevisiae
Concentration: 0.1 - 500 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: no data
Year: GLP: no
Test substance: other TS: no data
Reliability: (3) invalid
Remark: data are derived from reviews
24-APR-2001 (58)

5.6 Genetic Toxicity 'in Vivo'

Type: other
Species: rat Sex: male/female
Strain:
Route of admin.: oral unspecified
Exposure period: twice (1st, 3rd day of oestrus)
Doses: 2000 mg/kg bw
Result:
Method: other
Year: GLP: no data
Test substance: other TS: Santocure
Remark: incomplete and inexact data on study design
Result: No increased postimplantation embryonic mortality (= "index of mutagenicity").
Reliability: (3) invalid
Remark: unsuitable test system
24-APR-2001 (63)

5.7 Carcinogenicity

Species: mouse Sex: male/female
Strain: other: B6C3F1 and B6AKF1
Route of admin.: oral unspecified
Exposure period: 18 months
Frequency of treatment: daily
Post. obs. period: no
Doses: see remarks
Result: negative
Control Group: other: yes
Method: other
Year: GLP: no
Test substance: other TS: Durax
Remark: dose: 7th to 28th day of age: 215 mg/kg bw/d by stomach tube, thereafter administration of 692 mg/kg diet (app.: 99 mg/kg bw/d)
Result: no increased tumor incidence
Reliability: (2) valid with restrictions
Remark: deviations from standard guidelines are acceptable with regard to the creation date of the study
17-OCT-2001 (64) (65)

Species: mouse Sex: male/female
Strain: other: B6C3F1 and B6AKF1
Route of admin.: s.c.
Exposure period: 1 d
Frequency of treatment: once
Post. obs. period: 18 months
Doses: 1000 mg/kg bw
Result: negative
Control Group: other: yes
Method: other
Year: GLP: no
Test substance: other TS: Durax
Result: no increased tumor incidence
Reliability: (2) valid with restrictions
Remark: deviations from standard guidelines are acceptable with regard to the creation date of the study
17-OCT-2001 (64)

5.8 Toxicity to Reproduction

Type: Fertility
Species: rat Sex: female
Strain:
Route of admin.: oral feed
Exposure Period: day 0-20 of gestation
Frequency of treatment: daily
Duration of test:
Doses: 0, 0.001%, 0.01%, 0.1% and 0.5%.
Control Group: yes
NOAEL Parental: .01 %
NOAEL F1 Offspr.: .1 %
Method:
Year: GLP:
Test substance:
Result: Average daily intakes were 0, 0.7, 7.1, 69.6 and 288.8 mg/kg respectively. Significantly lower maternal body weight gain, food consumption and fetal body weight means were noted in the 0.5% group. Maternal body weight gains were significantly reduced in the 0.1% group. There were NO significant compound-related effects on pre- and post-implantation losses, the number and ratio of live to dead fetuses, or terata.
Flag: Critical study for SIDS endpoint
24-APR-2001 (66)

Type: other
Species: rat Sex: female
Strain: no data
Route of admin.: oral unspecified
Exposure Period: daily
Frequency of treatment: 1st to 3rd day of estrus
Duration of test:
Doses: 2000 mg/kg bw/d
Control Group: yes
NOAEL Parental: 2000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: Santocur
Remark: post observation period: up to the 19th day of pregnancy
Result: lowered weight of fetuses, no change in fertility, no visible signs of poisoning in dams
Reliability: (3) invalid
Remark: unsuitable test system
24-APR-2001 (63)

5.9 Developmental Toxicity/Teratogenicity

Species: rat Sex: female
Strain: other: Charles river COBS CD
Route of admin.: gavage
Exposure period: 6th to 15th day of pregnancy
Frequency of treatment: daily
Duration of test:
Doses: 100, 300, 500, 900 mg/kg bw/d
Control Group: yes
NOAEL Maternalt.: = 100 mg/kg bw
NOAEL Teratogen.: = 500 mg/kg bw
Method: OECD Guide-line 414 "Teratogenicity"
Year: 1981 GLP: yes
Test substance: other TS: N-cyclohexyl-2-benzothiazole; purity = 97%
Remark: 1) 100 mg/kg bw:
NOEL
2) 300 mg/kg bw:
maternal: body weight gain, decr.
3) 500 mg/kg bw:
maternal: alopecia; body weight gain, decr.;
body weight, decr.
offspring: fetus, weight, decr.;
NOEl, teratogenic effects
4) 900 mg/kg bw:
maternal: excessive toxicity; death
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
17-OCT-2001 (67)

Species: rat Sex: female
Strain: other: Institute's own breeding colony (Imp: DAK)
Route of admin.: gavage
Exposure period: days 6 to 15 of gestation
Frequency of treatment: once a day
Duration of test: day 20 of gestation
Doses: 50, 150 and 450 mg/kg
Control Group: yes, concurrent vehicle
NOAEL Maternalt.: 150 mg/kg bw
NOAEL Teratogen.: 50 mg/kg bw
Method: other
Year: GLP: no data
Test substance:
Result: 450 mg/kg: decreased body weight gain, increased relative kidney weights, decreased absolute spleen weights of the dams; 150 and 450 mg/kg: dose dependent increased number of fetuses with internal hydrocephalus; the number of fetuses with enlarged cerebral ventricles and/or renal pelvis was not dose dependendent increased
24-APR-2001 (68)

Species: rat Sex: female
Strain: Wistar
Route of admin.: oral feed
Exposure period: day 0 to day 20 of pregnancy
Frequency of treatment: daily
Duration of test:
Doses: 0.7; 7.1; 69.6 or 288.8 mg/kg bw/d
Control Group: yes
NOAEL Maternalt.: 69.6 mg/kg bw
NOAEL Teratogen.: 288.8 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: Soxinol CZ-G, 99 % pure
Remark: dose: 0.001; 0.01; 0.1 or 0.5 % in the diet
Result: except reduced food consumption, lowered weight of fetuses and of the placentae in the highest dosage group no sings of toxicity in any group; no embryotoxic or teratogenic effects
Reliability: (2) valid with restrictions
Remark: acceptable, well documented publication
24-APR-2001 (69)

Species: rat Sex: female
Strain:
Route of admin.: oral feed
Exposure period: days 6-15 of gestation
Frequency of treatment:
Duration of test:
Doses: 0, 100, 300, or 500 mg/kg
Control Group: yes
NOAEL Maternalt.: 300 mg/kg bw
NOAEL Teratogen.: 300 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: N-cyclohexyl-2-benzothiazole; purity = 97%
Result: Fetal body weight means and maternal body weight gains were significantly reduced in the high dosage groups.
Maternal general toxicity: None below 300 mg/kg
Foetal data: No effects below 300 mg/kg
24-APR-2001 (70)

Species: rat Sex: female
Strain: no data
Route of admin.: oral unspecified
Exposure period: daily
Frequency of treatment: 4th to 11th day of pregnancy
Duration of test:
Doses: 2000 mg/kg bw/d
Control Group: other: yes
Method: other
Year: GLP: no data
Test substance: other TS: Santocur
Remark: post exposure period: up to the 19th day of pregnancy
Result: lowered weight of fetuses, increased embryonic mortality, no visible signs of poisoning in dams, increased postimplantation embryonic mortality
Reliability: (3) invalid
Remark: unsuitable test system
24-APR-2001 (63)

Species: other Sex: no data
Strain:
Route of admin.:
Exposure period:
Frequency of
treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: The substance was injected into the heart of 3-day chicken embryos
Result: some malformations
Reliability: (3) invalid
Remark: test method not validated
24-APR-2001 (71)

Species: other Sex: no data
Strain:
Route of admin.:
Exposure period:
Frequency of
treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: 3-day old chicken embryos received a maximum dose of 1 mole/egg (injected into the air-chamber); the relevance of this test system in relation to mammals remains questionable
Result: 13 % malformed embryos
Reliability: (3) invalid
Remark: test method not validated
24-APR-2001 (72)

5.10 Other Relevant Information

Type: Metabolism
Remark: About 92% of the administred radioactivity was recovered from urin and feces within 3 days after administration of 14C-N-cyclohexyl-2-benzothiazol-sulfenamide. No specific organ affinity was observed. Metabolites were cyclohexylamine and 2-mercaptobenzothiazole.
Reliablity: 2
Remark: data are generally regarded as sufficient
Source: Bayer AG Leverkusen
24-NOV-1995 (73)

Type: other
Remark: in a 4-week comedogenicity (acnegenicity) assay, Santocure vulcanization accelerator was applied to the inner surface of rabbit ears 5 days per week at concentrations of 0.01, 0.1 or 10 % in chloroform; no production of comedones was observed after repeated treatment
Reliability: 3 GLP: No
Remark: International Protocol Compliance: No
Source: Monsanto
Bayer AG Leverkusen
23-APR-1996 (74)

Type: other
Remark: Reliability: 2
Remark: acceptable, well documented publication when MBT, MBTS, MMBT and CBS (= mercapto mix patch testing standard) were dissolved in petrolatum or in buffer of physilological pH, they were mainly converted into the redox pair MBT and MBTS
Source: Bayer AG Leverkusen
24-NOV-1995 (75)

Type: other: metabolism/pharmacokinetics
Remark: A single oral dose of 250 mg 14C-CBS/rat (3m): ca. 47% radioactivity in urine and 45 % in faeces (total recovery after 3 days=92%)
2h after administration no other metabolite than MBTS (65%) was observed in the stomach
Incubation with artifical gastric juice: Transformation to MBT and MBTS
Reliability: 3
Remark: poor or deficient study design
Source: Bayer AG Leverkusen
25-APR-1996 (76)

5.11 Experience with Human Exposure

Remark: Occupational exposure to Santocure has been reported to cause irritation to the eyes, skin and upper respiratory tract
Reliability: 2
Source: Monsanto
Bayer AG Leverkusen
26-APR-1996 (77)

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(77) Toxicology Profile Santocure Accelerator

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 102-77-2
CAS No.	102-77-2
EINECS Name	2-(morpholinothio)benzothiazole
EINECS No.	203-052-4
TSCA Name	Morpholine, 4-(2-benzothiazolylthio)-
Molecular Formula	C11H12N2OS2

Producer Related Part
Company:
Creation date: 15-JUL-1999

Substance Related Part
Company:
Creation date: 15-JUL-1999

Memo: Rubber and Plastic Additives (RAPA) HPV Panel

Printing date: 15-OCT-2001
Revision date:
Date of last Update: 15-OCT-2001

Number of Pages: 60

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: American Chemistry Council (formerly Chemical Manufacturers Association) Rubber and Plastic Additives (RAPA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States
Phone: 703-741-5600
Telefax: 703-741-6091

12-OCT-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

12-OCT-2001

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Country: United States

12-OCT-2001

Type: cooperating company
Name: Crompton Corporation
Country: United States

12-OCT-2001

Type: cooperating company
Name: Flexsys America L.P.
Country: United States

12-OCT-2001

Type: cooperating company
Name: Noveon, Inc (formerly BF Goodrich)
Country: United States

12-OCT-2001

Type: cooperating company
Name: R.T. Vanderbilt Company, Inc.
Country: United States

12-OCT-2001

Type: cooperating company
Name: The Goodyear Tire & Rubber Company
Country: United States

12-OCT-2001

Type: cooperating company
Name: The Lubrizol Corporation
Country: United States

12-OCT-2001

Type: cooperating company
Name: UOP, LLC.
Country: United States

12-OCT-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: solid
Purity: > 93 % w/w
20-OCT-1999

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

2-morpholinothio-benzothiazole
20-OCT-1999

N-oxydiethylene-2-benzothiazolesulfenamide
20-OCT-1999

1.3 Impurities

CAS-No: 110-91-8
EINECS-No: 203-815-1
EINECS-Name: morpholine
Contents: < .4 % w/w
Remark: others: disulphides and sulfonic acid derivatives of mercaptobenzothiazole, dimercaptobenzothiazole, and methylmercaptobenzothiazole < 6%
20-OCT-1999

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern

Type: type
Category: Use resulting in inclusion into or onto matrix
20-OCT-1999

Type: industrial
Category: Polymers industry
20-OCT-1999

Type: use
Category: Vulcanizing agents
20-OCT-1999

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value: 150.7 degree C
Method: other: MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Melting Point: 308.70 deg C (Adapted Joback Method)
Melting Point: 111.17 deg C (Gold and Ogle Method)
Mean Melt Pt : 209.94 deg C (Joback; Gold,Ogle Methods)
Selected MP: 150.68 deg C (Weighted Value)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

Value: 75 - 90 degree C
29-SEP-2000 (2)

Value: > 78 degree C
24-APR-2001 (3)

Value: 79 degree C
29-SEP-2000 (4)

2.2 Boiling Point

Value: 385.1 degree C
Method: other: MPBPWIN (v1.31) Adapted Stein and Brown Method
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

Value:
Decomposition: yes
Flag: Critical study for SIDS endpoint
15-OCT-2001 (3)

2.3 Density

Type: relative density
Value: 1.35 g/cm3 at 20 degree C
24-APR-2001 (3) (4)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: .000001346 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 385.05 deg C (estimated))
(Using MP: 150.68 deg C (estimated))
VP: 2.79E-007 mm Hg (Antoine Method)
VP: 1.01E-006 mm Hg (Modified Grain Method)
VP: 2.22E-006 mm Hg (Mackay Method)
Selected VP: 1.01E-006 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

Value: .0000023 hPa at 20 degree C
24-APR-2001 (3)

Value: .0000045 hPa at 25 degree C
24-APR-2001 (3)

2.5 Partition Coefficient

log Pow: 1.025 at 25 degree C
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

log Pow: 3.49
Method:
Year:
Testsubstance: other TS: Santocure MOR Accelertor
Remark: Pow: 3100
Flag: Critical study for SIDS endpoint
15-OCT-2001 (5)

2.6.1 Water Solubility

Value: 3061 mg/l at 25 degree C
Method: other: WSKOW (v1.36)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

Value: 32 other: ppm
Qualitative: not soluble
Testsubstance: other TS: Sanatocure MOR Accelerator
15-OCT-2001 (6)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: 188 degree C
Type: open cup
Method: other: DIN 51584
Year:
24-APR-2001 (3)

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 156000 molecule/cm3
Rate constant: .0000000001199482 cm3/(molecule * sec)
Degradation: 50 % after 1.1 hour(s)
Deg. Product: not measured
Method: other (calculated): AOP Program (v1.89)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

Type: water
Light source: Sun light
Spectr.of subst.: lambda (max, >295nm): 300 nm
Conc. of subst.: 1.006 mg/l at 26 degree C
DIRECT PHOTOLYSIS
Halflife t1/2: 1 hour(s)
Degradation: 97 % after 4 hour(s)
Method: other (measured): Method similar to ASTM draft methd No. 6, ASTM E35.24 Subcommittee Aqueous Photolysis Task Group
Year: 1980 GLP: no data
Test substance: other TS: Santocure MOR
Remark: Dark control recovery was 97 % at 4 hours while Santocurs MOR values at 0, 1, 2, 3 and 4 hours were 100 %, 45 %, 15 %, 8 % and 3 %, respectively.
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
24-APR-2001 (7)

3.1.2 Stability in Water

Type: abiotic
Degradation: 24 % after 25 hour(s)
at pH 7
Method: other: Hydrolysis in pH buffered dionized water
Year: 1984 GLP: yes
Test substance: other TS: Santocure MOR
Remark: Primary purpose of this study was to identify hydrolysis by products. After 7 days of exposure to pH 7 water the following by products were determined to be present in the percentages listed in parenthesis: benzothiazole (64 %), mercaptobenzothiazole (21 %), unknown with proposed composition of C11H14S2N2O2 (15 %) proposed structure shown below and morpholine (% not listed). Hydrolysis was complete after 7 days at pH 7.
Reliability: (1) valid without restriction
GLP study; Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
15-OCT-2001 (8)

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air, watr, soil, sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: (calculation) EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	9.47e-005	2.14	1000	2.15e-015
Water	44.6	900	1000	1.19e-016
Soil	55.3	900	1000	4.06e-015
Sediment	0.0904	3.6e+003	0	1.09e-016

Persistence Time: 823 hr
Reaction Time: 1.3e+003 hr
Advection Time: 2.24e+003 hr
Percent Reacted: 63.3
Percent Advected: 36.7
Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 100 mg/l related to COD (Chemical Oxygen Demand)
Degradation: 0 % after 28 day
Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"
Year: 1988 GLP: no
Test substance: other TS: 2-morpholinothio-benzothiazole; purity > 93%
Reliability: (1) valid without restriction
Meets National standards method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (3)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: ThOD: 1880 mg/g
24-APR-2001 (3)

3.7 Bioaccumulation

Species: other
Exposure period:
Concentration:
BCF: 1.23
Elimination:
Method: other: BCF Program (v2.13)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Result: Log Kow (estimated) : 1.02
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 1.02

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70

Estimated Log BCF = 0.089 (BCF = 1.227)
Reliability: (2) valid with restrictions
Accepted calculation method

15-OCT-2001 (1)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type:	static
Species:	Pimephales promelas (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: no
NOEC:	= 1
LC50:	= 3.5
Method:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year:	1984 GLP: yes
Test substance:	other TS: Santocure MOR
Remark:	C.I. for 96 h LC50 = 2.7-4.4 mg/l; 24 and 48 h LC50 = 4.0 mg/l
Test condition:	length = 25.8 mm; weight = 0.26 g
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

15-OCT-2001 (9)

Type:	
Species:	Lepomis macrochirus (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	Analytical monitoring: yes
LC50:	11.5
Method:	other: Standard Methods for the Examination of Water and Wastewater, 13th ed., American Public Health Association
Year:	1971 GLP: no data
Test substance:	other TS: Delac MOR
Result:	LC50 (96 hrs) = 11.5 ppm
Test condition:	The fish (1-3 inches in length) were obtained from a state licensed commercial fish hatchery and were retained for at least 10 days before use. The dilution water was natural pond water with a hardness expressed as 44 ppm CaCO3. A saturated aqueous extract (SAE) was made by allowing the material to sit in distilled water after vigorous shaking for at least 24 hours. The SAE was filtered and then tested. All tests were conducted at room temperature (22 degrees C), pH 6.5-8.5 and all DO's remained above 4mg/l at all times during a test.
Reliability:	(1) valid without restriction Meets National standards method (AFNOR/DIN)
Flag:	Critical study for SIDS endpoint

15-OCT-2001 (10)

Type: other: calculation
Species: other: Fish
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 1560.288
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
15-OCT-2001 (1)

Type: other: calculation
Species: other: Saltwater Fish
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 222.538
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
15-OCT-2001 (1)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 1
LC100: 5
Method:
Year: 1989 GLP: no
Test substance:
Remark: The substance was given in water and stirred for 24 h on a magnetic stirrer: at all concentrations undissolved particles remained in the medium.
24-APR-2001 (3)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: = 4.4
Method: other: Bionomics Lab protocol; see test conditions
Year: 1976 GLP: no data
Test substance: other TS: as prescribed by chapter 1 Monsanto
Remark: C.I. for 96 h LC50 = 3.6 - 5.6; 24 h LC50 >7.5 mg/l; 48 h LC50 = 6.0 mg/l
Test condition: carrier-acetone; 15l water; 10 fish/treatment; no aeration; 22 degrees C
24-APR-2001 (11)

Type: static
Species: Oncorhynchus kisutch (Fish, fresh water, marine)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
LC0: >= 10
Method:
Year: GLP: no
Test substance:
Remark: length: 5 - 10 cm; loss of equilibrium occured in 7 - 11 h; only concentration tested
24-APR-2001 (12)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: = .56
LC50: = 1.4
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 GLP: yes
Test substance: other TS: as prescribed by chapter 1 Monsanto
Remark: C.I. for LC50 = 1-1.8 mg/l; 24 h LC50 = 1.5 mg/l; 48 h LC50 = 1.4 mg/l
Test condition: hardness 40-45 mg/l CaCO3
24-APR-2001 (13)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: = 1.3
Method: other: Bionomics Lab protocol; see test conditions
Year: 1976 GLP: no data
Test substance: other TS: as prescribed by chapter 1 Monsanto
Remark: C.I. = 97-1.8 mg/l; 24 h LC50 = 5.3 mg/l; 48 h LC50 = 1.4 mg/l
Test condition: Carrier-acetone; 15 l water; 10 fish/treatment; length = 2.7 cm; no aeration; 12 degrees C
24-APR-2001 (11)

Type: static
Species: Oncorhynchus tschawytscha (Fish, fresh water, marine)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
LC0: >= 10
Method:
Year: GLP: no
Test substance:
Remark: length: 5 - 10 cm; only concentration tested
24-APR-2001 (12)

Type: static
Species: Ptychocheilus oregonensis (Fish, fresh water)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
LC0: >= 10
Method:
Year: GLP: no
Test substance:
Remark: length: 5 - 10 cm; only concentration tested
24-APR-2001 (12)

Type:
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: Analytical monitoring: no
Method:
Year: 1988 GLP: no
Test substance:
Remark: The substance was eluted in the concentration 1 g/l for 2 h, filtered and the filtrate tested (DOC of the filtrate: 11 mg/l)
LC0 at dilution 1:8
LC100 at dilution 1:2
24-APR-2001 (3)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: = 1
EC50: = 4
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 GLP: no data
Test substance: other TS: Santocure MOR
Remark: C.I. for EC50 = 2.9-5.4; 24 h EC50 = 6.8 mg/l
Source: MonsantoBayer AG Leverkusen
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
15-OCT-2001 (14)

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: = 1
EC50: = 4.5
Method: other: EPA. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians, EPA-660/3-75-009
Year: 1975 GLP: no data
Test substance: other TS: Santocure MOR
Remark: C.I. for 48 h EC50 = 3-6.8 mg/l; 24 h EC50 = 13 mg/l
Source: MonsantoBayer AG Leverkusen
Test condition: static, 250 ml water; 19 degrees C; 16 h light
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
15-OCT-2001 (15)

Type:
Species: other: Paratanytareum parthenogenetica
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: = 1.8
EC50: = 5.3
Method: other: EPA. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians, EPA-660/3-75-009
Year: 1975 GLP: yes
Test substance: other TS: Santocure MOR
Remark: C.I. for 48 h EC50 = 4.5-6.2 mg/l; 25 h EC50 = 8.6 mg/l
Source: MonsantoBayer AG Leverkusen
Test condition: static; 20 degrees C; 200 ml water; 16 h light
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
15-OCT-2001 (16)

Type: other: calculation
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
LC50 : 1562.446
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
15-OCT-2001 (1)

Type: other: calculation
Species: Mysidopsis bahia (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50 : 905.743
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
15-OCT-2001 (1)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: green algae
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 923.219
ChV : 52.399
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
15-OCT-2001 (1)

Species: other aquatic plant
Endpoint: other: cell number
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 2
Method:
Year: GLP:
Test substance:
08-OCT-2001

Species: other aquatic plant
Endpoint: other: chlorophyll a
Exposure period: 96
Unit: mg/l Analytical monitoring:
EC50: 2
Method:
Year: GLP:
Test substance:
08-OCT-2001

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: > 10000
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: 1988 GLP: no
Test substance:
Remark: direct weight
Reliability: (1) valid without restriction
Meets National standards method
15-OCT-2001 (3)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type: other
Species: Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint:
Exposure period: 14 day
Unit: other: mg/l
LC50: 3110.605
Method: other:ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
15-OCT-2001 (1)

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of Animals: 16
Vehicle: other: corn oil
Value: 12560 mg/kg bw
Method: other: Industrial BIO-TEST Laboratories, Inc.
Year: 1974 GLP: no
Test substance: other TS: OBTS, purity = 90-94%
Method: Industrial BIO-TEST Laboratories, Inc.
Initial scrrening was conducted to determine general level of toxicity.
2 rats/sex/dose were administered the test material by gavage. The rats were then housed individually and observed for 14 days. Initial and final body weights, mortalities and reactions were recorded. A necropsy examination was conducted on all animals.

The acute oral median lethal dose was calculated using the techniques of Weil CS (1952); Thompson WR (1947) and Thompson WR and Weil CS (1952).
Result: Adverse reactions observed at
4556 mg/kg: hyporeactivity and ruffed fur;
6834 mg/kg: as above plus salivation and labored breathing;
10250 mg/kg: as above plus muscular weakness, prostration, diuresis

Dose level (mg/kg)	mortality rate	% mortality
4556	0/4	0
6834	0/4	0
10250	1/4	25
15380	3/4	75

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
15-OCT-2001 (17)

Type: LD50
Species: rat
Strain: Wistar
Sex: male/female
Number of Animals: 20
Vehicle: other: propylene glycol
Value: > 10000 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: Delac MOR
Method: The test material was given as a 33% (w/v) suspension in propylene glycol to groups of 10 males and 10 femaels in a single dose of 30 ml/kg bw (10g test material/kg bw). The rats received feed and water ad libitum during the 14 day observation period. The rats were observed for intoxication and mortality. All animals were necropsied.
Result: None of the treated animals showed any reaction upon treatment. No deaths occurred during the observation period. Macroscopic examination did not reveal treatment-related alterations.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
15-OCT-2001 (18)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 1980 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
06-APR-1992 (19)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 7940 mg/kg bw
Method:
Year: GLP:
Test substance:
Remark: mortality: 0/7
Reliability: (2) valid with restrictions
15-OCT-2001 (20)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method:
Year: GLP:
Test substance:
Remark: mortality: 0/10
Source: Bayer AG Leverkusen
06-APR-1992 (21)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 1870 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (22)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 1980 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (23)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 4000 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (24)

Type: LD100
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 4000 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (23)

Type: LDLo
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 250 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (23)

Type: other: LD
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 3980 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (20)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Strain:
Sex: male
Number of
Animals: 10
Vehicle:
Exposure time: 1 hour(s)
Value: > 151 mg/l
Method: other: according to the technique specified in the Regulations (Federal Register, August 12, 1961)
Year: 1961 GLP: no
Test substance: other TS: OBTS; purity not noted

Result: Two rats died on the 4th or 10th day post-exposure. No other mortalities occurred.

During the one-hour exposure, animals generally exhibited excessive preening and masticatory movements, excessive salivation, and occasional periods of excited activity.

Signs of toxicity prior to the mortalities were depression, depresed righting and placement reflexes, ataxia (1 animal-4th day post exposure) and diarrhea stains of 2 day duration (1 animal -10th day post exposure).

Surviving rats exhibited normal appearance and behavior throughout the 14-day observation period.

Test condition: Sample was ground in a blender and filtered through a 40-mesh screen; then generated as a dust for exposure.

Reliability: (1) valid without restriction
Meets National standards method

Flag: Critical study for SIDS endpoint

15-OCT-2001 (25)

Type: LC0
Species: rat
Strain:
Sex: male/female
Number of Animals: 20
Vehicle: other: undiluted powder
Exposure time: 4 hour(s)
Value: ca. .09 mg/l
Method: other: Industrial Bio-Test Laboratories protocol
Year: 1974 GLP: no
Test substance: as prescribed by 1.1 - 1.4

Method: Ten albino rats were exposed to the dust of the test material for four hours in a 70 liter chamber. The concentration was determined by sampling the test atmosphere in the breathing zone of the animals, collected on a glass fiber filter. The average filter concentration was 0.09 mg/l air. The exposed animals and 10 untreated controls were observed for 14 days.

Result: There were no deaths during the exposure or 14-day observation period. All rats in the treated and control groups gained weight during the study. There were no gross pathologic findings attributable to inhalation of the test material. Gross pathologic changes in test and untreated contrtol animals were essentially the same.

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment

Flag: Critical study for SIDS endpoint

15-OCT-2001 (26)

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rabbit
Strain:	New Zealand white
Sex:	male/female
Number of Animals:	4
Vehicle:	other: neat
Value:	> 3000 mg/kg bw
Method:	
Year:	GLP: no
Test substance:	other TS: OBTS
Method:	Young adult New Zealand albino rabbits were acclimated and examined prior to testing. Twenty-four hours prior to testing, the backs of the animals (approx 30% total body surface) were shaved free of hair. The material was applied at the highest reasonable dosage and the test site was covered with plastic sheeting. After 24 hours the plastic sheeting and residual material were removed. The animals were examined for local skin reactions, behavioral abnormalities and mortality for 14 days. Initial, 7 and 14 day body weights were recorded. A necropsy was conducted on all animals.
Result:	mortality = 0/4
Test condition:	The test material was applied as received to abraded, pre-moistened skin.
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag:	Critical study for SIDS endpoint

15-OCT-2001 (17)

Type:	LD50
Species:	rabbit
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	> 7940 mg/kg bw
Method:	
Year:	GLP:
Test substance:	

24-APR-2001 (27)

Type: other: LD
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 3980 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (28)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.p.
Value: ca. 100 - 200 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (29)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.p.
Value: = 100 mg/kg bw
Method:
Year: GLP:
Test substance:
24-APR-2001 (30)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: other: no data
Value: = 3150 mg/kg bw
Method:
Year: GLP:
Test substance:
Remark: sex: male
24-APR-2001 (31)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: other: no data
Value: = 3000 mg/kg bw
Method:
Year: GLP:
Test substance:
Remark: sex: female
24-APR-2001 (31)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration: undiluted

Exposure: Occlusive
Exposure Time: 24 hour(s)
Number of
Animals:
PDII: .8
Result: slightly irritating
EC classificat.: not irritating
Method: Draize Test
Year: GLP: no data
Test substance: other TS: OBTS; purity not noted
Method: dose: 0.5 g undiluted applied to intact and abrdaded skin; occluded for 24 hours.
Result:

sample tested	Primary Irritation Score
OBTS 1-A	0.1
OBTS 1-B	0.2
OBTS 1-C	0.1
OBTS 1-D	0.8

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
15-OCT-2001 (17)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals: 12
PDII:
Result: slightly irritating
EC classificat.:
Method:
Year: GLP:
Test substance: other TS: Delac MOR
Result: The test substance caused very slight skin irritation in 2 of 12 rabbits.
15-OCT-2001 (32)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: 24 hours
Year: GLP:
Test substance:
Remark: score: 0.6/8.0, practically non-irritating
15-OCT-2001 (27)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: 500 mg/animal, 2 animals, onto the skin of the ear for 24 h (semi-occlusive), test substance removed with water at the end of exposure; post exposure period of 7 d
Year: GLP:
Test substance:
Remark: the same procedure with a test substance of different

origin came to the result: slight skin irritant
24-APR-2001 (33)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: test substance was applied to the clipped, intact skin (occlusive) and removed after 24 h with water, observation over several days, the data were scored according to the method of Draize
Year: GLP:
Test substance:
24-APR-2001 (28)

Species: guinea pig
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result:
EC classificat.:
Method: other: 0.5, 2, 5 and 10 % being tested to determine the threshold irritation concentration, application over 24 h (semi-oclusive), readings were performed at 1, 24 and 48 h after removal
Year: GLP:
Test substance:
Remark: result: 5 and 10 % produced irritant reactions
Source: Bayer AG Leverkusen
15-OCT-1993 (34)

5.2.2 Eye Irritation

Species: rabbit
Concentration: undiluted
Dose: 100 other: mg
Exposure Time:
Comment: not rinsed
Number of Animals: 24
Result: moderately irritating
EC classificat.: irritating
Method: Draize Test
Year: GLP: no data
Test substance: other TS: OBTS; purity not noted
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
15-OCT-2001 (17)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals: 6
Result: moderately irritating
EC classificat.: irritating
Method:
Year: GLP:
Test substance: other TS: Delac MOR
Result: The test substance caused moderate ocular lesions in 4 of 6 rabbits.
15-OCT-2001 (32)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: slightly irritating
EC classificat.:
Method: other: 24 hours
Year: GLP:
Test substance:
Remark: score: 6.0/110.0
15-OCT-2001 (27)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method: other: 100mg/24h
Year: GLP:
Test substance:
Remark: result: moderate
24-APR-2001 (35)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: slightly irritating
EC classificat.:
Method: other: 50 mg/animal, 2 animals, instillation into the conjunctival sac, post exposure period of 7 d
Year: GLP:
Test substance:
Remark: the same procedure with a test substance of different origin came to the result: moderate eye irritant
24-APR-2001 (33)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: slightly irritating
EC classificat.:
Method: other: finely ground test substance were placed in the conjunctival sac, the eyes were rinsed after 24 h, the data scored according to the method of Draize
Year: GLP:
Test substance:
24-APR-2001 (28)

5.3 Sensitization

Type: other: see remarks
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method: other: a modification of Buehler's method
Year: GLP:
Test substance:
Remark: cross-sensitivity: 8/10 sensitized animals showed a positive reaction with MBT
15-OCT-2001 (34)

Type: other: see remarks
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method: other: closed epicutaneous test (no further information)
Year: GLP:
Test substance:
Remark: result: 8/12 animals positive (challenge with 0.5M)
1/12 animals positive (challenge with 0.05M)
15-OCT-2001 (36)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: 4/31 rubber contact dermatitis patients had a positive patch test result
15-OCT-2001 (36)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: 17/17 subjects allergic to MBT were positive in the test with MBS; the test with MBS was negative in 20 controls
15-OCT-2001 (37)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: 24/49 individuals showed a positive patch test reaction during the induction phase (for the challenge applications, petrolatum alone was applied in lieu of test sample)
24-APR-2001 (38)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: Repeat patch testing with 1 or 10 % Santocure MOR resulted in sensitization reactions in 7/24 and 28/31 subjects, respectively. Recrystallized Santocure MOR showed only 1/20 individuals being affected.
15-OCT-2001 (39)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: Evaluation of Santocure MOR, mercaptobenzothiazole, morpholine and two oxidized impurities, the sulfonamide and the sulfenamide, were tested in vitro with lymphocytes from sensitized individuals to determine if DNA synthesis/stimulation would result. The results showed the oxidized contaminants to be primarily responsible for the sensitization response.
15-OCT-2001 (40)

Type: other: in vitro lymphocyte assay
Species:
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: An in vitro lymphocyte assay was performed to determine if Santocure MOR or process contaminants might possess the ability to induce delayed type hypersensitivity. Based on the data, it appears that Santocure MOR is not a sensitizer, but two potential process contaminants may be.
24-APR-2001 (41)

5.4 Repeated Dose Toxicity

Species:	rat	Sex:	
Strain:			
Route of admin.:	oral feed		
Exposure period:	4 w		
Frequency of treatment:			
Post. obs. period:			
Doses:	100, 200, 500, or 1000 mg/kg bw/d		
Control Group:			
NOAEL:	200 mg/kg bw		
LOAEL:	500 mg/kg bw		
Method:			
Year:		GLP:	
Test substance:	other TS: Santocure MOR		
Result:	Body weight reductions were noted in animals at 500 and 1000 mg/kg. Increased liver and kidney weights were observed in the high-dose males		
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment		
Flag:	Critical study for SIDS endpoint		

15-OCT-2001 (42)

Species:	rat	Sex:	male/female
Strain:	other: Charles River CD strain		
Route of admin.:	oral feed		
Exposure period:	113 weeks		
Frequency of treatment:	daily		
Post. obs. period:			
Doses:	5, 50, 400 mg/kg bw/d		
Control Group:	yes		
NOAEL:	5 mg/kg bw		
LOAEL:	50 mg/kg bw		
Method:	other: according to Hazelton Laboratories Europe Ltd.		
Year:	1982	GLP:	no data
Test substance:	other TS: Santocure MOR		
Result:	50 and 400 mg/kg bw: reductions in body weight gain and food consumption; dose related increases in kidney and liver weights; no other evidence of chronic toxicity		
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment		
Flag:	Critical study for SIDS endpoint		

15-OCT-2001 (43)

Species: rat
Sex:
Strain:
Route of admin.: inhalation
Exposure period: 4 w
Frequency of treatment: 6 h/d at 5 d/w
Post. obs. period:
Doses: 4.4, 9.8, and 10.2 mg/m3
Control Group:
NOAEL: 9.8 mg/m³
Method:
Year:
GLP:
Test substance:
Result: Santocure MOR caused slight irratation in exposed animals. Slight body weight reductions and reductions in lung weights were observed in males of high-exposure group. Histopathological examination revealed no alterations in the tissues of the high-exposure group animals. Slight depressions in blood glucose and elevations in SGOT values were found in animals at all exposure levels, but these findings were not associated with the presence of any tissue lesions.
The no effect level for this study was considered to be 9.8 mg/m3.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
15-OCT-2001 (44)

Species: rabbit
Sex:
Strain:
Route of admin.: dermal
Exposure period: 21 d
Frequency of treatment:
Post. obs. period:
Doses: 125, 500, 2000
Control Group:
NOAEL: 2000
Method:
Year:
GLP:
Test substance:
Result: Repeated applications of Santocure MOR produced no evidence of toxicity related to test material administration. Only a slight degree of dermal irritation was noted.
15-OCT-2001 (44)

Species: mouse Sex: male/female
Strain: other: Slc:ddY
Route of admin.: oral feed
Exposure period: 3 months
Frequency of treatment: no data
Post. obs. period: no data
Doses: 0.012, 0.046, 0.188, 0.75 % (18, 69, 282, 1125 mg/kg bw)
Control Group: no data specified
NOAEL: 282 mg/kg bw
LOAEL: 1125 mg/kg bw
Method:
Year: GLP:
Test substance:
Result: 0.75 % group: decreased body weight gain, slightly increased levels of GPT and kidney weights (no further information)
15-OCT-2001 (31)

Species: rat Sex: no data
Strain: no data
Route of admin.: inhalation
Exposure period: 15 d
Frequency of treatment: 2h/d
Post. obs. period:
Doses: 0.3 - 0.4 mg/l
Control Group: no data specified
Method:
Year: GLP:
Test substance:
Remark: no detailed information; evaluation impossible
Result: no change in body weight; the working of the nervous system was affected
Reliability: (4) not assignable
Documentation insufficient for assessment
15-OCT-2001 (23)

Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 56 d
Frequency of treatment: daily, 7d/w
Post. obs. period: 2w
Doses: 125, 250, 500 mg/kg bw
Control Group: yes, concurrent vehicle
Method:
Year: GLP:
Test substance:
Result: mean body weight and mean body weight gain did not reveal any significant effect in any of the dose groups; tissue-to-body weight ratios were normal except an increase in the stomach/body weight ratio (125, 250 mg/kg bw); no abnormalities in selected animals during gross pathological examination
24-APR-2001 (45)

Species: mouse Sex: male/female
Strain: other: Slc:ddY
Route of admin.: oral feed
Exposure period: 21 months
Frequency of treatment: no data
Post. obs. period: no data
Doses: 0.01, 0.1, 1 %
Control Group: no data specified
NOAEL: 150 mg/kg bw
LOAEL: 1500 mg/kg bw
Method:
Year: GLP:
Test substance:
Remark: doses: 15, 150, 1500 mg/kg bw
remarks: see also chapter 5.7
Result: 1 % group: decreased body weight gain (no further information)
15-OCT-2001 (31)

Species: mouse Sex: no data
Strain: other: Slc:ddY
Route of admin.: dermal
Exposure period: 21 months
Frequency of treatment: no data
Post. obs. period: no data
Doses: 10 % suspended in olive oil
Control Group: no data specified
NOAEL: 10 %
Method:
Year: GLP:
Test substance:
Result: no compound related adverse effects (no further information)
15-OCT-2001 (31)

Species: rabbit Sex: no data
Strain: no data
Route of admin.: oral unspecified
Exposure period: 3.5 months
Frequency of treatment: on alternative days (2 months), daily (1.5 months)
Post. obs. period: no data
Doses: 20 mg/kg bw
Control Group: no data specified
Method:
Year: GLP:
Test substance:
Remark: no detailed information; evaluation impossible
Result: general conditions were unchanged; the pigmentary function (?) of the liver was affected; changes in the liver, kidneys and lung were observed
24-APR-2001 (23)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: <= 500 ug/ml
Cytotoxic Conc.: >= 500 ug/plate
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: GLP: yes
Test substance: other TS: Three sample comparison (two comercial: OBTS and NOBS; and OBTS 4X recrystallized sample)
Reliability: (1) valid without restriction
GLP guideline study

Flag: Critical study for SIDS endpoint
15-OCT-2001 (46)

Type: Mammalian cell gene mutation assay
System of testing: CHO cells
Concentration: 0.1, 0.3, 1.0, 3.0, 10, 30, 50, 100, 150, 300 ug/ml
Cytotoxic Conc.: >=150 ug/ml (with and without activation)
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year: 1983 GLP: yes
Test substance: other TS: Commercial and purified OBTS
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
15-OCT-2001 (47)

Type: Mammalian cell gene mutation assay
System of testing: mouse lymphona cells L 5158 TK+/-
Concentration: <= 50.0 mg/plate
Cytotoxic Conc.: > 50 ug/ml
Metabolic activation: with and without
Result: positive
Method: OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year: 1981 GLP: yes
Test substance: other TS: Three sample comparison (two comercial: OBTS and NOBS; and OBTS 4X recrystallized sample)
Result: An analysis of small vs. large colonies was not made, however because the lower-limit cutoff on the colony counter is 0.3mm, it is assumed that the mutation response was mainly due to large colonies.

The assay was positive for all three test substances under conditions of metabolic activation.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
15-OCT-2001 (46)

Type: Sister chromatid exchange assay
System of testing: CHO cells
Concentration: 1,5,10,20,40 ug/ml (non-activated) 5,10,15,30,60 ug/ml (activated)
Cytotoxic Conc.: >= 50 ug/ml
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 479 "Genetic Toxicology: In vitro Sister Chromatid Exchange Assay in Mammalian Cells"
Year: 1984 GLP: yes
Test substance: other TS: OBTS commercial and purified
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
15-OCT-2001 (48)

Type: Cytogenetic assay
System of testing: CHO cells
Concentration: <= 10 mg/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1979 GLP:
Test substance: other TS: purity = 90-95 %
Remark: GLP: Signed Quality Assurance Inspection Statement
Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
15-OCT-2001 (49)

Type: other: Cell Transformation Assay
System of testing: BALB / 3T3 Cell line
Concentration: <= 30.0 mg/l
Cytotoxic Conc.:
Metabolic activation: without
Result: negative
Method: other
Year: 1981 GLP:
Test substance: other TS: Three sample comparison (two comercial: OBTS and NOBS; and OBTS 4X recrystallized sample)
Remark: GLP: Signed Quality Assurance Inspection Statement
Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
15-OCT-2001 (50)

Type: other: DNA repair assay
System of testing: E. coli W3110 (pol A+) E. coli W3078 (pol A-)
Concentration: <= 1.0 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1979 GLP:
Test substance: other TS: 90-95 %
Remark: GLP: Signed Quality Assurance Inspection Statement
Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
15-OCT-2001 (51)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: <= 5.0 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: 1979 GLP:
Test substance: other TS: OBTS; purity =90-95 %
Remark: GLP: Signed Quality Assurance Inspection Statement
Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
15-OCT-2001 (49)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: <= 1000 ug/plate
Cytotoxic Conc.: >= 100 ug/plate
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: 1982 GLP: no data
Test substance: other TS: OBTS; purity > 99 %
Method: The standard Ames protocol was followed with the following exception: instead of duplicate plates for the positive controls, in trial #1, one of the plates contained twice the standard dose.
Reliability: (1) valid without restriction

Meets generally accepted scientific method and is described in sufficient detail
15-OCT-2001 (52)

Type: Bacterial gene mutation assay
System of testing: Salmonella typhimurium TA 100, TA 98
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
15-OCT-2001 (53)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
15-OCT-2001 (54)

Type: Ames test
System of testing: Salmonella typhimurium TA 1535, TA 1537, TA 98, TA 100
Concentration:
Cytotoxic Conc.:
Metabolic activation: with
Result: negative
Method:
Year: GLP:
Test substance:
15-OCT-2001 (55) (56)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1976 GLP:
Test substance:
15-OCT-2001 (57)

Type: Mammalian cell gene mutation assay
System of testing: CHO cells
Concentration: 2.5 - 50 ug/ml
Cytotoxic Conc.: >=40 ug/ml
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year: 1986 GLP:
Test substance: other TS: OBTS commercial: purity = 94.12%, purified: purity >= 99%
Remark: GLP: Signed Quality Assurance Inspection Statement
commercial and purified sample
Reliability: (1) valid without restriction
Guideline study
15-OCT-2001 (58)

Type: Mammalian cell gene mutation assay
System of testing: mouse lymphoma cells L5178Y TK+/-
Concentration: <= 50.0 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method: other
Year: 1979 GLP:
Test substance: other TS: 90-95 % purity
Remark: GLP: Signed Quality Assurance Inspection Statement
result: significant increases in the mutation frequency were observed in the absence and presence of rat liver S9 metabolic activation
Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
15-OCT-2001 (49)

Type: Mammalian cell gene mutation assay
System of testing: mouse lymphoma cells L5178Y TK+/-
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method:
Year: GLP:
Test substance:
Remark: result: significant increases in the mutation frequeny were only observed in the presence of rat liver S9 metabolic activation
15-OCT-2001 (59)

Type: other: Cell transformation assay
System of testing: BALB/3T3 Cell line
Concentration: <= 35.0 mg/l
Cytotoxic Conc.:
Metabolic activation: without
Result: positive
Method: other
Year: 1979 GLP:
Test substance: other TS: 90-95 %
Remark: GLP: Signed Quality Assurance Inspection Statement
Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
15-OCT-2001 (49)

Type: Yeast gene mutation assay
System of testing: Saccharomyces cerevisiae D4
Concentration: <= 1.0 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: 1979 GLP:
Test substance: other TS: 90-95 %
Remark: GLP: Signed Quality Assurance Inspection Statement
15-OCT-2001 (51)

Type: Yeast gene mutation assay
System of testing: Saccharomyces cerevisiae D4
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
15-OCT-2001 (57)

Type: other: DNA repair assay
System of testing: E. coli W1310 (polA+), E. coli p3478 (polA-)
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 472 "Genetic Toxicology: Escherichia coli Reverse Mutation Assay"
Year: GLP:
Test substance: other TS: Three sample comparison (two comercial: OBTS and NOBS; and OBTS 4X recrystallized sample)
Reliability: (1) valid without restriction
Guideline study
15-OCT-2001 (60)

Type: other: DNA repair suspension assay
System of testing: E. coli W3110 (pol A+) E. coli P3078 (pol A-)
Concentration: <= 2.5 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method: other
Year: 1981 GLP:
Test substance: other TS: 90-95 % purity
Remark: GLP: Signed Quality Assurance Inspection statement
Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
15-OCT-2001 (49)

5.6 Genetic Toxicity 'in Vivo'

Type: Dominant lethal assay
Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 56d
Doses: 125, 250, 500 mg/kg bw
Result: negative
Method: other
Year: 1980 GLP: yes
Test substance: other TS: 90-95 % purity
Remark: see also chapter 5.4
Result: no dominant lethal mutations
Reliability: (1) valid without restriction
GLP study; Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
15-OCT-2001 (45)

Type: Dominant lethal assay
Species: rat Sex: male/female
Strain:
Route of admin.: oral unspecified
Exposure period: up to 3d
Doses: 200 mg/kg bw
Result:
Method:
Year: GLP:
Test substance:
Remark: no further information
Result: An increase in total embryonic mortality in treated females and in females mated with treated males.
15-OCT-2001 (61)

Type: unspecified
Species: Drosophila melanogaster Sex: no data
Strain:
Route of admin.: other
Exposure period: no data
Doses: no data
Result:
Method:
Year: GLP:
Test substance:
Result: Not described in detail.
Opinion of the author:MBS showed a weak mutagenic activity.
15-OCT-2001 (62)

5.7 Carcinogenicity

Species:	mouse	Sex:	
Strain:			
Route of admin.:	gavage		
Exposure period:	79 w		
Frequency of treatment:			
Post. obs. period:			
Doses:	90 mg/kg/d		
Result:	negative		
Control Group:			
Method:			
Year:		GLP:	
Test substance:	other TS: N-oxydiethylene-2-benzothiazole sulfenamide (NOBS)		
Result:	No adverse effects were reported, and no statistically significant increase in tumor incidences were observed in the study.		

25-APR-2001 (63)

Species:	rat	Sex:	no data
Strain:	no data		
Route of admin.:	oral feed		
Exposure period:	2 years		
Frequency of treatment:			
Post. obs. period:			
Doses:	5, 50, 400 mg/kg bw/d		
Result:	negative		
Control Group:	no data specified		
Method:			
Year:		GLP:	
Test substance:			
Remark:	no further information; see also chapter 5.4		
Result:	no evidence of oncogenicity		

15-OCT-2001 (64)

Species: mouse Sex: male/female
Strain: other: Slc:ddY
Route of admin.: oral feed
Exposure period: 21 months
Frequency of treatment: no data
Post. obs. period: no data
Doses: 0.01, 0.1, 1 %
Result: negative
Control Group: no data specified
Method:
Year: GLP:
Test substance:
Remark: doses: 15, 150, 1500 mg/kg bw
remarks: see also chapter 5.4
Result: histopathologically no compound related nonneoplastic or neoplastic lesions (no further information)
15-OCT-2001 (31)

Species: mouse Sex: male/female
Strain: other: (C57BL/6 x C3H/Anf)Fl and (C57BL/6 x AKR)Fl
Route of admin.: oral unspecified
Exposure period: 18 months
Frequency of treatment: daily
Post. obs. period: no
Doses: 464 mg/kg bw (days 7-28 of age); 1492 ppm (after 28 days of age)
Result: negative
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: doses: 1492 ppm = dosage in diet = approx. 224 mg/kg bw
Result: no significant indication of tumorigenicity after oral administration
25-APR-2001 (65)

Species: mouse Sex: male/female
Strain: other: (C57BL/6 x C3H/Anf)Fl abd (C57BL/6 x AKR)Fl
Route of admin.: s.c.
Exposure period: 1d
Frequency of treatment: once
Post. obs. period: 18 months
Doses: 464 mg/kg bw
Result: negative
Control Group: yes
Method:
Year: GLP:
Test substance:
Result: no significant indication of tumorigenicity
15-OCT-2001 (66)

Species: mouse Sex:
Strain:
Route of admin.: s.c.
Exposure period:
Frequency of treatment: single injection
Post. obs. period: 78 w
Doses: 1000 mg/kg
Result: negative
Control Group:
Method:
Year: GLP:
Test substance: other TS: N-oxydiethylene-2-benzothiazole sulfenamide (NOBS)
Result: No adverse effects were reported, and no statistically significant increase in tumor incidences were observed in the study.
15-OCT-2001 (63)

5.8 Toxicity to Reproduction

Type:
Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure Period: 56d
Frequency of
treatment: daily, 7d/w
Duration of test:
Doses: 125, 250, 500 mg/kg bw
Control Group: yes, concurrent vehicle
Method:
Year: GLP:
Test substance:
Remark: see also chapter 5.4
post observation period: 2w
Result: pregnancy rates of the dose groups were comparable to those of the controls
25-APR-2001 (45)

Type:
Species: rat Sex: male/female
Strain:
Route of admin.: gavage
Exposure Period: 3d
Frequency of
treatment: 1st and 3rd days of estrus (female); twice an interval of 3d
Duration of test:
Doses: 200 mg/kg bw
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: The object of the investigations was to study the level of the embryonic mortality (EM).
post observation period: till 19th day of pregnancy
Result: no visible signs of poisoning; changes in the estrous cycle; delay to conceptions; decreased fetus wieghts; increased total embryonic mortality (EM) with normal postimplantation EM
25-APR-2001 (67)

5.9 Developmental Toxicity/Teratogenicity

Species: rat Sex: female
Strain: other: Charles River
Route of admin.: oral unspecified
Exposure period: 6 - 15 gestation day
Frequency of treatment: daily
Duration of test: until 20 gestation day
Doses: 100, 300, 1000 mg/kg bw
Control Group: yes
NOAEL Maternalt.: 300 mg/kg bw
NOAEL Teratogen.: 1000 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: Santocure MOR
Remark: Maternal toxicity was noted at the highest dose level.
Result: no teratogenic response was observed (no further information)
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
15-OCT-2001 (68)

Species: rat Sex: female
Strain: no data
Route of admin.: oral feed
Exposure period: day 0 through 20 of gestation
Frequency of treatment:
Duration of test:
Doses: 0.02, 0.5 % (13, 270 mg/kg bw/d)
Control Group: yes
NOAEL Maternalt.: 270 mg/kg bw
NOAEL Teratogen.: 270 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: Santocure MOR
Remark: no further information
Result: no teratogenic, fetotoxic or maternally toxic effects
25-APR-2001 (27)

Species: rat Sex: female
Strain:
Route of admin.: gavage
Exposure period: 2d
Frequency of
treatment: 4th and 11th days of pregnancy
Duration of test: till 19th day of pregnancy
Doses: 200 mg/kg bw
Control Group: other: yes
Method:
Year: GLP:
Test substance:
Remark: The object of the investigations was to study the level of the embryonic mortality (EM).
Result: no visible signs of poisoning; decreased fetus weights; increased total embryonic mortality (EM) with normal postimplantation EM
25-APR-2001 (67)

Species: rat Sex: female
Strain: other: wistar
Route of admin.: oral feed
Exposure period: day 0 of gestation to day 21 postparturition
Frequency of
treatment:
Duration of test:
Doses: 0.02, 0.5 %
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: doses: 3.9 and 81 mg/rat/day (calculated by the author)
Result: There were no harmful effects on the fetuses with respect to external, skeletal and visceral anomalies; the stillborn litter number tended to increase; the postnatal development of the off- spring was normal
25-APR-2001 (69)

Species: rat Sex:
Strain:
Route of admin.: oral feed
Exposure period: d 0 to 21 of gestation
Frequency of
treatment: daily
Duration of test:
Doses: 13 or 270 mg/kg/d
Control Group:
Method:
Year: GLP:
Test substance: other TS: N-oxydiethylene-2-benzothiazole sulfenamide (NOBS)
Result: no adverse effect on fetal or postnatal development
25-APR-2001 (70)

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of
treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: method: test compounds were tested for embryotoxicity and induction of malformations on three-day chicken embryos
Result: increased frequency of malformations
25-APR-2001 (71) (72)

5.10 Other Relevant Information

Type: Biochemical or cellular interactions
Remark: the conjugation between MBS and lysine, cysteine, and glyzine was confirmed
Source: Bayer AG Leverkusen
20-OCT-1993 (73)

Type: other
Remark: Intratracheal injection of MBS powder caused pathological alterations in the lungs (interstitial productive process, emphysema, bronchitis)
Source: Bayer AG Leverkusen
07-APR-1992 (74)

Type:
Remark: Generation date of chap. 5: March 1992
Source: Bayer AG Leverkusen
20-OCT-1993

5.11 Experience with Human Exposure

26-MAY-1994

(1) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

(2) Uniroyal Chemical MSDS

(3) Bayer AG data

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7.1 End Point Summary

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7.2 Hazard Summary

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7.3 Risk Assessment

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